BZ 35 (MASTER INDEX) (1984) December 1984 ISSN 0010-4655

# Computer Physics Communications

An international journal devoted to computational physics and computer programs in physics

## MASTER INDEX VOLUMES 1–30

July 1969–December 1983

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**Published monthly**

**Printed in The Netherlands**

# COMPUTER PHYSICS COMMUNICATIONS

# Computer Physics Communications

**Editor**

K.V. ROBERTS
*Culham Laboratory, Abingdon*

**Volume 35 (1984)**

**Master Index Volumes 1–30**

**July 1969–December 1983**

EUROPHYSICS JOURNAL

NORTH-HOLLAND – AMSTERDAM

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# PREFACE

This volume contains the indexes for papers and authors, and summaries for the programs which have been published in volumes 1–30 of Computer Physics Communications (CPC). The first issue of the journal appeared in 1969 and volume 30 was completed in December 1983. Hence this volume contains a complete summary of CPC over its first 15 years.

It was stated in the first issue of CPC that the aim of the journal was to facilitate the exchange of physics programs and relevant information about the use of computers in the physics community. To meet this need CPC has published two classes of papers:

(i) papers in the general area of computational physics concerned with computational methods and the applications of computers to physics,

(ii) summaries and long write-ups describing programs held in the CPC international physics Program Library at the Queen's University of Belfast together with program adaptions and erratum notices.

The CPC Program Library has been described in Comput. Phys. Commun. 19 (1980) 11–15 and now contains over 800 programs. Request forms for individual programs or for a subscription to the whole library are given in this volume.

In conclusion, Miss C. Jackson is to be thanked for preparing all the computerised indexes in this volume.

November 1984

P.G. BURKE

# CONTENTS AND LAYOUT OF MASTER INDEX (VOLUMES 1–30)

This Master Index to volumes 1–30 of the journal Computer Physics Communications is made up of four main sections as follows:

A. Subject index to the Computational physics papers
B. Program index
C. Program summaries
D. Author index
CPC Program Library; description, charges, subscription and order forms

The contents and layout of each of the four sections of the index are described in more detail below.

## A. Subject index to Computational physics papers p.p. A-1–A-21

This index gives a guide to the subjects of all papers published within the *Computational physics* section of CPC (volumes 1–30). The *Main subject headings* used in the index (together with the page numbers where they first appear) are listed below. Most main subject headings are further subdivided into relevant topics as indicated in the *Key to entries in subject index A*, shown below.

*Main subject headings*

| *Page* | *Subject* |
|---|---|
| A-1 | Astronomy and Astrophysics |
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*Key to entries in subject index A*

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4 47 Simple Monte Carlo simulation for solving methodological problems of detecting the extensive air showers electron component. T. Stanev.
③ ④ ⑤

① Main subject.
② Subdivision of the Main subject.
③ Volume number (3s is supplement to volume 3).
④ Page number of article.
⑤ Title of article. Author(s).

## B. Program index p.p. B-1–B-75

The program index gives a guide to the material that has appeared in the *Computer programs in physics* section of CPC (volumes 1–30). The *Main subject headings* used to divide up the index (together with the page numbers where the subject headings first appear) are listed below. Main subjects are frequently further subdivided into relevant topics as indicated in the *Key to entries in program index B*, shown below.

Each entry in the index, in addition to giving the program name, the title and place of appearance of the original article describing the program, also lists the subroutines used by the program and (when relevant) refers the reader to other versions of the same program.

### *Main subject headings*

| *Page* | *Subject* | *Page* | *Subject* | *Page* | *Subject* |
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②— **Theoretical Methods (see also Computational Methods) (cont.)**

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| ③ | ④ | ⑤ | ⑥ | ⑦ |

① Main subject.
② Subdivision of the Main subject.
③ Volume number of article.
④ Page number of article.
⑤ Page number in the section "Program summaries" (index C) of the present master index.
⑥ Catalogue number of the CPC Program Library.
⑦ Title of the program (Programming Language). Title of paper. Author(s).
If appropriate, subroutines required by the program and other versions of the program are also given.
Corrections (erratum notices) and Adaptations belonging to a program follow the entry of that program.

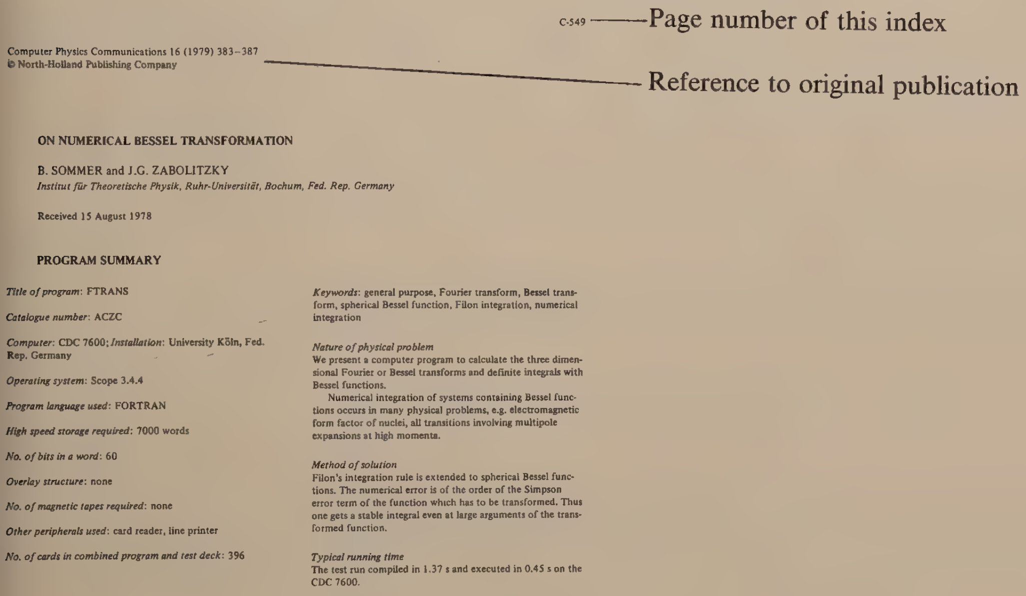
## C. Program summaries

This section of the master index reproduces the program summaries of all articles that have appeared in the *Computer programs in physics* section of CPC (volumes 1–30). The summaries appear here in the same running order as the original articles. The location of a particular program summary can be found either by reference to the *Program index* (section B) or if the author's name(s) are known, by means of the *Author index* (section D).

At the top left hand corner of each program summary there is a source reference line, giving the volume number, year of publication and page numbers of the original article, as indicated on the example below.

It should be noted that on pages containing a group of erratum notices or a program summary and erratum notice(s), the source reference line applies to the first notice or the program summary on the page. Subsequent notices appear in the same volume as the first article but sometimes on later pages.

*Example of entry in section C*



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Computer Physics Communications 16 (1979) 383–387
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——Reference to original publication

ON NUMERICAL BESSEL TRANSFORMATION

B. SOMMER and J.G. ZABOLITZKY
*Institut für Theoretische Physik, Ruhr-Universität, Bochum, Fed. Rep. Germany*

Received 15 August 1978

PROGRAM SUMMARY

*Title of program*: FTRANS

*Catalogue number*: ACZC

*Computer*: CDC 7600; *Installation*: University Köln, Fed. Rep. Germany

*Operating system*: Scope 3.4.4

*Program language used*: FORTRAN

*High speed storage required*: 7000 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 396

*Keywords*: general purpose, Fourier transform, Bessel transform, spherical Bessel function, Filon integration, numerical integration

*Nature of physical problem*
We present a computer program to calculate the three dimensional Fourier or Bessel transforms and definite integrals with Bessel functions.

Numerical integration of systems containing Bessel functions occurs in many physical problems, e.g. electromagnetic form factor of nuclei, all transitions involving multipole expansions at high momenta.

*Method of solution*
Filon's integration rule is extended to spherical Bessel functions. The numerical error is of the order of the Simpson error term of the function which has to be transformed. Thus one gets a stable integral even at large arguments of the transformed function.

*Typical running time*
The test run compiled in 1.37 s and executed in 0.45 s on the CDC 7600.

## D. Author index

This author index covers all articles appearing in volumes 1–30 of Computer Physics Communications. As shown on the *Key to entries in author index D* below, those entries relating to articles which original appeared in the *Computer programs in physics* section of the journal have a cross reference to section C of the present master index. This gives the page number in section C where the relevant program summary appears.

*Key to entries in author index D*

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| ① | ② | ③ | ④ | ⑤ |

① Volume number.
② Page number.
③ Page number in section C: Program summaries.
④ Author.
⑤ Title of paper; in case of an Erratum notice also the reference to the original paper is given.

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| 12 | 335 | **C–408** ACIB | 0001 CALCULATE LATERAL RANGES (Fortran). Adaptation of a program for depth distribution of energy deposition by ion bombardment: calculation of ion lateral ranges. I. Manning, M. Rosen and J.E. Westmoreland. |
| 12 | 339 | **C–408** ACIB | 000ACORRECTION 21/09/75 (Fortran). Depth distribution of energy deposition by ion bombardment. (C.P.C. 7(1974)85). I. Manning and G.P. Mueller. |
| 12 | 339 | **C–408** ACIB | 000BCORRECTION 5/03/75 (Fortran). Depth distribution of energy deposition by ion bombardment. (C.P.C. 7(1974)85). I. Manning and G.P. Mueller. |
| 7 | 401 | **C–255** AAGX | POSITRONFIT EXTENDED (Fortran). POSITRONFIT EXTENDED: a new version of a program for analysing positron lifetime spectra. P. Kirkegaard and M. Eldrup. See other versions of this program AAGK 3(1972)240, AAGZ 13(1977)371, AAHI 15(1978)97, AANN 23(1981)307, ACKX 30(1983)359. |
| 13 | 203 | **C–425** ACMN | KRONIG (Fortran). Numerical solution of Kramers–Kronig transforms by a Fourier method. S.J. Collocott. |
| 17 | 393 | **C–567** ACMN | 0001 TRAPZAL (Fortran). Adaptation: numerical solution of the Kramers–Kronig transforms by trapezoidal summation as compared to a Fourier method. S.J. Collocott and G.J. Troup. |
| 13 | 371 | **C–438** AAGZ | DBLCON (Fortran). DBLCON: a version of POSITRONFIT with non–Gaussian prompt for analysing positron lifetime spectra. W.K. Warburton. See other versions of this program AAGK 3(1972)240, AAGX 7(1974)401, AAHI 15(1978)97, AANN 23(1981)307, ACKX 30(1983)359. |

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| 15 | 97 | **C–485** | AAHI | INTERACTIVE POSITRONFIT (Fortran). INTERACTIVE POSITRONFIT: a new version of a program for analysing positron lifetime spectra. C.J. Virtue, R.J. Douglas and B.T.A. McKee. See other versions of this program AAGK 3(1972)240, AAGX 7(1974)401, AAGZ 13(1977)371, AANN 23(1981)307, ACKX 30(1983)359. |
| 21 | 91 | **C–652** | ACUF | EXAFS 1,2,3,4,5 (Fortran). Fourier analysis of EXAFS data, a self–contained Fortran program package. E. Indrea and N. Aldea. |
| 23 | 307 | **C–732** | AANN | PATFIT (Fortran). Program system for analysing positron lifetime spectra and angular correlation curves. P. Kirkegaard, M. Eldrup, O.E. Mogensen and N.J. Pedersen. See other versions of this program AAGK 3(1972)240, AAGX 7(1974)401, AAGZ 13(1977)371, AAHI 15(1978)97, ACKX 30(1983)359. |
| 25 | 193 | **C–781** | AARR | DLXANES (Fortran). Calculation of X–ray absorption near edge structure, XANES. P.J. Durham, J.B. Pendry and C.H. Hodges. |
| 30 | 359 | **C–922** | ACKX | PFPOSFIT (Fortran). PFPOSFIT: a new version of a program for analysing positron lifetime spectra with non–Gaussian prompt curve. W. Puff. See other versions of this program AAGK 3(1972)240, AAGX 7(1974)401, AAGZ 13(1978)371, AAHI 15(1978)97, AANN 23(1981)307. |

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| 2 | 11 | **C–58** | ACMD | SYMMETRY AND BAND STRUCTURE 1 (Fortran). Selection of reciprocal lattice vectors. V. Hoffstein and O. Moller. |
| 2 | 17 | **C–59** | ACME | SYMMETRY AND BAND STRUCTURE 2 (Fortran). Storage and retrieval of group theoretical information. V. Hoffstein and O. Moller. |
| 2 | 26 | **C–60** | ACMF | SYMMETRY AND BAND STRUCTURE 3 (Fortran). Construction of symmetrized Hamiltonian matrix. V. Hoffstein and O. Moller. Subroutine required by this program is ACME 2(1971)17. |
| 3 | 88 | **C–127** | ACMI | GROUP THEORY OF LATTICE DYNAMICS (Fortran). Group–theoretical analysis of lattice vibrations. See erratum Comp. Phys. Commun. 4(1972)382. T.G. Worlton and J.L. Warren. See other version of this program ACMM 8(1974)71. |
| 4 | 249 | **C–157** | ACMI | 0001 EXTERNAL MODES (Fortran). External modes of molecular crystals. T.G. Worlton. |
| 6 | 149 | **C–215** | ACMI | 0002 IMR CALCULATION (Fortran). Irreducible multiplier representations. T.G. Worlton. |
| 8 | 141 | **C–269** | ACMI | B00ACORRECTION TO 0002 04/08/74 (Fortran). Irreducible multiplier representations. (C.P.C.6(1973)149). T.G. Worlton. |
| 4 | 361 | **C–162** | ACMJ | SYMMETRIZED APW (Fortran). Symmetrized program for calculating energy bands and electronic structure of solids. V. Hoffstein, D.K. Ray and M. Belakhovsky. |
| 10 | 67 | **C–328** | ACMJ | 0001 SYMMETRY AND BANDSTRUCTURE (Fortran). Symmetry and bandstructure. J.Th.M. de Hosson. |
| 8 | 71 | **C–262** | ACMM | GROUP THEORY LATTICE DYNAMICS 2 (Fortran). Improved version of group–theoretical analysis of lattice dynamics. J.L. Warren and T.G. Worlton. See other version of this program ACMI 3(1972)88. |
| 9 | 231 | **C–304** | ACUA | SPACE GROUP REPRESENTATIONS (Fortran). Numerical calculations of the irreducible representations of space groups. N. Neto. |

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| 10 | 104 | **C–331** | ACKJ | NORMAL COORDINATE ANALYSIS (Fortran). Normal coordinate analysis of crystals. J.Th.M. de Hosson. |
| 14 | 193 | **C–461** | ACXQ | FYCOOR (Fortran). I. A computer program for generation of a complete set of coordinates and force matrices for normal mode calculations of crystals and molecules. F.Y. Hansen. Subroutines required by this program are ACXR 14(1978)219, ACXS 14(1978)245. |
| 14 | 219 | **C–462** | ACXR | FYFRE (Fortran). II. A program for computing normal modes of molecules, crystal phonon dispersion relations and structure factors for neutron inelastic scattering. F.Y. Hansen. Subroutines required by this program are ACXQ 14(1978)193, ACXS 14(1978)245. |
| 17 | 423 | **C–571** | ACXR | 000A CORRECTION 22/12/78 (Fortran). II. A program for computing normal modes of molecules, crystal phonon dispersion relations and structure factors for neutron inelastic scattering. (C.P.C. 14(1978)219). F.Y. Hansen. |
| 14 | 245 | **C–464** | ACXS | FYADJ (Fortran). III. A force constant adjuster program to obtain a least squares fit to observed frequencies of molecules and crystals. F.Y. Hansen. Subroutines required by this program are ACXQ 14(1978)193, ACXR 14(1978)219. |

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 10-14. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# GINZBURG-LANDAU-FLUXOIDS

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Received 18 March 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): Ginzburg-Landau-Fluxoids

*Catalogue number*: ACKA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: Telefunken TR4. *Installation*: Rechenzentrum Stuttgart, Germany

*Operating system or monitor under which the program is executed*: MV 11

*Programming languages used*: ALGOL 60

*High speed store required*: 4058 words. *No. of bits in a word*: 52

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? None

*No. of cards in combined program and test deck*: 235

*Keywords descriptive of problem and method of solution*: Ginzburg-Landau-Theory, Fluxoids, Finite Difference-Method.

*Nature of physical problem*

The Ginzburg-Landau-equations are solved for a straight single fluxoid containing an (integer) number $q$ of flux quanta, starting from an approximate solution which has to be submitted by the user if $q > 1$.

*Method of solution*

An iteration procedure is applied based on successive linearizations of the Ginzburg-Landau-equations. In each iteration step, the system of linearized differential equations is solved by a finite-difference-technique with small intervals near the core and big intervals far outside. The line-energy of the fluxoid is calculated.

*Typical running time*

If one takes about one hundred lattice points ranging from a radial distance $r = 0$ to about $r = 7$ (reduced units of the Ginzburg-Landau-theory), and if an absolute error of the modulus of the order parameter and of the magnetic field of less than $10^{-3}$ is required, typical running times on the Telefunken TR4 are about 3 minutes, including compilation time (about 1 minute).

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 15-20. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# FRACTIONAL PARENTAGE COEFFICIENTS FOR EQUIVALENT p SHELL AND EQUIVALENT d SHELL ELECTRONS

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*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, Northern Ireland*

Received 22 March 1969

## PROGRAM SUMMARY (p SHELL ELECTRONS)

*Title of program* (32 characters maximum): P SHELL C. F. P.

*Catalogue number*: ACQB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL 1907; 1900 SERIES. *Installation*: Queen's University, Belfast, Northern Ireland

*Operating system or monitor under which the program is executed*: QUBE

*Programming languages used*: FORTRAN

*High speed store required*: 2,880 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 173

*Keywords descriptive of problem and method of solution*: Atomic, Nuclear, Racah C. F. P.

### *Nature of physical problem*

The subroutine CFPP evaluates the Racah coefficient [1,2] of fractional parentage for equivalent p shell electrons. These are defined by $(p^n L S \,|\}\, p^{n-1} L' S', p L S)$ where $n$ denotes the number of equivalent electrons and $L$, $S$; $L'$, $S'$ are respectively the angular momentum and spin quantum numbers of the state in question and its parent state.

### *Method of solution*

Since any state of a $p^n$ multiplet may be completely specified by the two quantum numbers $L$ and $S$, it is possible to set up two two-dimensional arrays $L_{ij}$ and $S_{ij}$, where the subscript $i$ refers to the number of electrons and the subscript $j$ refers to a label which denotes a particular allowed combination of $L$ and $S$ values.

If the state in question is identified by the labels $n$ and $j_1$ then its parent state can be identified by the labels $(n-1)$ and $j_2$ where $j_2$ refers to a particular allowed combination of $L$ and $S$ values for the $p^{n-1}$ configuration. The labels $n$, $j_1$ and $j_2$ may then be used to define a unique element of a table $T_n(j_1,j_2)$ where $n$ refers to a particular table, $j_1$ to a row index and $j_2$ to a column index. This is the required fractional parentage coefficient.

### *Typical running time*

$\ll 1$ second for one fractional parentage coefficient.

### *Unusual features of program*

If the state in question or its parent state is forbidden on account of an incorrect combination of $L$ and $S$ values then an erroneous value (in practice 9.9) is given to the fractional parentage coefficient. This may be replaced by an error statement if required.

The program CFPP shares its long write-up with CFPD, a similar program for d shell coefficients of fractional parentage.

### *References*

[1] G. Racah, Phys. Rev. 63 (1943) 367.
[2] J. C. Slater, Quantum theory of atomic structure, Vol. 2 (McGraw-Hill, New York, 1960).

## PROGRAM SUMMARY (d SHELL ELECTRONS)

*Title of program* (32 characters maximum): D SHELL C. F. P.

*Catalogue number*: ACQC

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL 1907; 1900 SERIES. *Installation*: Queen's University, Belfast, Northern Ireland.

*Operating system or monitor under which the program is executed*: QUBE

*Programming languages used*: FORTRAN

*High speed store required*: 5,120 words. *No. of bits in a word*: 24

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 275

*Keywords descriptive of problem and method of solution*: Atomic, Nuclear, Racah C. F. P.

*Nature of physical problem*

The subroutine CFPD evaluates the Racah coefficient [1,2] of fractional parentage for equivalent d shell electrons. These are defined by $(\mathrm{d}^n VLS\,|\}\,\mathrm{d}^{n-1} V'L'S', \mathrm{d}LS)$ where $n$ denotes the number of equivalent electrons and $V, L, S$; $V', L', S'$ are respectively the seniority, angular momentum and spin quantum numbers of the state in question and its parent state.

*Method of solution*

Since any state of a $\mathrm{d}^n$ multiplet may be completely specified by the three quantum numbers $V$, $L$ and $S$, it is possible to set up three two-dimensional arrays $V_{ij}$, $L_{ij}$ and $S_{ij}$, where the subscript $i$ refers to the number of electrons and the subscript $j$ refers to a label which denotes a particular allowed combination of $V$, $L$ and $S$ values.

If the state in question is identified by the labels $n$ and $j_1$ then its parent state can be identified by the labels $(n-1)$ and $j_2$ where $j_2$ refers to a particular allowed combination of $V$, $L$ and $S$ values for the $\mathrm{d}^{n-1}$ configuration. The labels $n$, $j_1$ and $j_2$ may then be used to define a unique element of a table $T_n(j_1, j_2)$ where $n$ refers to a particular table, $j_1$ to a row index and $j_2$ to a column index. This is the required fractional parentage coefficient.

*Typical running time*

≪ 1 second for one fractional parentage coefficient.

*Unusual features of program*

If the state in question or its parent state is forbidden on account of an incorrect combination of $V$, $L$ and $S$ values then an erroneous value (in practice 9.9) is given to the fractional parentage coefficient. This may be replaced by an error statement if required

The program CFPD shares its long write-up with CFPP, a similar program for p shell coefficients of fractional parentage.

*References*

[1] G. Racah, Phys. Rev. 63 (1943) 367.
[2] J. C. Slater, Quantum theory of atomic structure, Vol. 2 (McGraw-Hill, New York, 1960).

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 21-24. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# A PROGRAM TO CALCULATE FRANCK-CONDON FACTORS

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*Cambridge, Massachusetts* 02138, *USA*

Received 18 March 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): FRANK-CONDON FACTOR PROGRAM

*Catalogue number*: AACA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6400; ANY CDC 6000 SERIES. *Installation*: Smithsonian Astrophysical Obs., Cambridge, Mass., USA

*Operating system or monitor under which the program is executed*: SCOPE

*Programming languages used*: FORTRAN

*High speed store required*: 15,600 words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 537

*Keywords descriptive of problem and method of solution*: Atomic, Structure, Transition, Franck-Condon, Bound States, Eigenvalues, Eigenfunctions, Schrödinger eq., Potential, Local, Numerov.

*Nature of physical problem*

Franck-Condon factors, $q_{v''v'}$, occupy an important role in the study of absorption and emission processes between discrete vibrational levels of two electronic states of a molecule [1]. They are defined by

$$q_{v''v'} = \left| \int \chi_{v''}(R)\,\chi_{v'}(R)\,\mathrm{d}R \right|^2 ,$$

where $\chi_{v''}(R)$, $\chi_{v'}(R)$ are the normalised wavefunctions associated with the vibrational levels $v''$, $v'$ of the lower and upper states, respectively.

*Method of solution*

The above problem involves the calculation of eigenvalues and eigenfunctions of the Schrödinger equation for two different potential functions. We have used the method of Mayers [2], which gives accurate eigenvalues and eigenfunctions from a resonable initial estimate of the eigenvalue. The equations have been solved numerically using Numerov's method [3] in a form developed by Allison [4].

*Restrictions on complexity*

The program can be easily modified to accept potential functions of any complexity rather than the analytical expression required by this version.

*Typical running time*

Best time: 555 Franck-Condon factors in 283 s.
Test time: 4 Franck-Condon factors in 5 s.

*Unusual features of program*

A single array of mesh points is used for the numerical integration corresponding to both upper and lower state wavefunctions. It is easy to invent a pathological case for which, with reference to a particular computer word length, integration of both equations using a single set of mesh points would not be possible. However, this situation did not occur in any of the cases we considered.

*References*

[1] R.W.Nicholls, Astrophys. J. 141 (1965) 819.
[2] D.F.Mayers, Numerical solution of ordinary and partial differential equations, ed. L.Fox (Pergamon Press, London-New York, 1962).
[3] D.R.Hartree, The calculation of atomic structures (John Wiley, New York, 1957).
[4] A.C.Allison, Ph. D. Thesis, Glasgow University (1967).

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 25-30. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# COULOMB FUNCTIONS FOR COMPLEX ENERGIES *

Taro TAMURA and Frank RYBICKI
*Center for Nuclear Studies, University of Texas, Austin, Texas, USA*

Received 20 May 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum) COULOM

*Catalogue number*: ABOC

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: University of Texas Computer Center

*Operating system or monitor under which the program is executed*: CDC Scope

*Programming languages used*: FORTRAN IV

*High speed store required*: 6550 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card reader, Lineprinter for driver

*No. of cards in combined program and test deck*: 547

*Keywords descriptive of problem and method of solution*: Nuclear, Schrödinger Eqn., Reactions, Scattering, Wave function, Gamow function, Coulomb, Complex Coulomb, Potential, Complex gamma function.

*Nature of physical problem*

Subroutine COULOM is a FORTRAN IV subroutine to calculate the regular and irregular Coulomb functions and their derivatives for a complex energy $E$. This subroutine can be called with the following three quantities as input: $L_{\max}$, the maximum value of the orbital angular momentum; $\eta$, the complex Coulomb parameter, and $\rho$, the complex wave number times the radius. This subroutine may be used, for example, in calculating the wave function (Gamow function) that describes the decay of a nucleus by emitting a charged particle, tunneling through or going over the Coulomb barrier. In this case the imaginary parts of $E$, $k$, and $\eta^{-1}$ are all negative. COULOM can, however, also be used if the imaginary parts of these quantities are positive or vanishing.

*Method of solution*

The method of calculation employed follows very closely that of Buck et al. [1], who adapted the general method of Fröberg [2] to nuclear problems limited to the case of real energy. Fröberg's formalism, however, works as well for complex $E$ as it does for real $E$. Therefore, having a subroutine for the Coulomb functions for real $E$, a subroutine for complex $E$ can be obtained by simply declaring most of the variables to be complex. The quantity $\sigma_0$, the complex Coulomb phase shift for the s-wave, needed in applying the method of ref. [1], is obtained in COULOM by using the formula $\exp(2i\sigma_0) = \Gamma(1+i\eta)/\Gamma(1-i\eta)$ and by calling GAMMA, a subroutine which calculates the complex $\Gamma$-function for complex arguments.

*Restrictions on the complexity of the problem*

This program may be used for a wide range of parameters that satisfy the condition $|\rho| \gg |\eta^2|$. Even if this condition is violated, the program may be used with somewhat reduced accuracy.

*Typical running time*

The typical running time for $L_{\max} \approx 10$ is of the order of one-tenth of a second on the CDC 6600 computer.

*References*

[1] B. Buck, R. N. Madison and P. E. Hodgson, Phil. Mag. 5 (1960) 118.
[2] C. E. Fröberg, Rev. Mod. Phys. 27 (1955) 399.

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* Work partially supported by the U.S. Atomic Energy Commission.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 31-34. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# A PROGRAM TO CALCULATE RADIATIVE RECOMBINATION COEFFICIENTS OF HYDROGENIC IONS

D. R. FLOWER and M. J. SEATON
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Received 27 May 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): HYDROGENIC RECOMBINATION COEFFS

*Catalogue number*: ACQD

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/65. *Installation*: University College London

*Operating system or monitor under which the program is executed*: SYSTEM/360

*Programming languages used*: FORTRAN IV

*High speed store required*: 1851 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader, Line Printer

*No. of cards in combined program and test deck*: 306

*Keywords descriptive of problem and method of solution*: Atomic, Astrophysics, radiative recombination, hydrogenic ions, asymptotic expansion, Kramers-Gaunt factor.

*Nature of physical problem*

Radiative recombination coefficients are required for various problems in physics and astrophysics; one such problem is the calculation of the ionization equilibria and recombination spectra of gaseous nebulae [1,2]. It is desirable that the calculation of these coefficients should be completely automatic. A program has therefore been written to calculate the coefficients $\alpha_n(Z, T)$ for radiative recombination to energy levels of principal quantum number $n$ of hydrogenic ions, $Z$ being the nuclear charge and $T$ the electron temperature. The program also calculates sums of recombination coefficients from $n = n''$ to $n = \infty$. It should be noted that hydrogenic data may be used to obtain a good approximation to the recombination coefficient of non-hydrogenic ions, summed over excited states [3].

*Method of solution*

The recombination coefficients are expressed as integrals over the photo-ionization cross-sections, which are evaluated using the first three terms in the asymptotic expansion of the Kramers-Gaunt $g$-factor [4]. The program is based on Seaton's paper [4], to which the reader is referred for a more detailed discussion of the method. The accuracy of the final results is determined by the approximation used for the $g$-factor and not by the numerical methods employed in the program. For $(T/Z^2) \leq 2 \times 10^4\,{}^\circ$K the maximum error in $\alpha_1$ will be 2.5% and the error $\alpha_n$ for $n > 1$ will be less than 1%. The accuracy becomes less good for higher temperatures.

*Restrictions on the complexity of the problem*

It should be noted that the program does *not* compute coefficients, $\alpha_{nl}$, for recombination on to individual $nl$ states but computes only total coefficients, $\alpha_{nl}$, for each value of $n$. Values of $\alpha_{nl}$ are tabulated by Burgess [5].

*Typical running time*

The complete program required 12 s to compile and 1.5 s to execute the section of the test run reproduced below.

*References*

[1] D. R. Flower, Astrophysical Letters 2 (1968) 205.
[2] M. J. Seaton, Monthly Notices Roy. Astron. Soc. 119 (1959) 90.
[3] A. Burgess and M. J. Seaton, Monthly Notices Roy. Astron. Soc. 121 (1960) 76.
[4] M. J. Seaton, Monthly Notices Roy. Astron. Soc. 119 (1959) 81.
[5] A. Burgess, Mem. Roy. Astron. Soc. 69 Part 1 (1964) 1.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 35-53. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# COMPUTATION OF TOTAL, DIFFERENTIAL, AND DOUBLE-DIFFERENTIAL CROSS SECTIONS FOR COMPOUND NUCLEAR REACTIONS OF THE TYPE (a, b), (a, b$\gamma$) AND (a, b$\gamma$-$\gamma$)

## (II) GENERALIZED PROGRAMS "MANDY" AND "BARBARA" FOR ARBITRARY ANGULAR MOMENTA IN HAUSER-FESHBACH-MOLDAUER FORMALISM

Eric SHELDON and Richard Michael STRANG
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Received 27 May 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): MANDY

*Catalogue number*: ABOA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: Burroughs B5500. *Installation*: University of Virginia, Charlottesville, Virginia, USA

*Operating system or monitor under which the program is executed*: Mark VIII

*Programming languages used*: ALGOL

*High speed store required*: 9000 words. *No. of bits in a word*: 48

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? B124 Card Reader; B321 Line Printer

*No. of cards in combined program and test deck*: 1233.

*Keywords descriptive of problem and method of solution*: Nuclear, Reaction, Mechanism, Angular Distribution, Statistical, Compound Nucleus, Differential Cross Section, Total Cross Section, Hauser-Feshbach, Satchler, Moldauer, Level-Width Fluctuation, Spin-Parity, Multipolarity, Mixing Ratio, Racah Functions, Clebsch-Gordan Coefficient, Racah Coefficient, [Wigner 3-*j* and 6-*j* Symbols], Legendre Polynomials, Transmission Coefficients, Penetrability, Spin-Orbit Coupling, Optical Potential, Compound-Elastic Scattering, Inelastic Scattering, Compound Stripping, Spin Assignments.

*Nature of physical problem*

Evaluation of total and differential cross sections in absolute and normalized form for angular distributions in low-energy nuclear reactions of the type (a, b), (a, b$\gamma$) or (a, b$\gamma\gamma$) according to statistical compound-nucleus theory in *j-j* coupling formalism. The program represents a generalization of an earlier version [1] in as much as the collision partners may each have arbitrary spin, mass, and relative orbital momentum; the emergent $\gamma$-radiations may be of pure or mixed multipolarity and provision is made for arbitrarily many extra exit channels of any given spin and orbital angular momentum. Spin-orbit interaction can be taken into consideration and, at option, the calculation can be made to proceed with and/or without the Moldauer level-width fluctuation modification and to extend automatically over a permuted range of spins and parities. It has been used not only for the analysis of inelastic nucleon distributions [1] but also for (d, p), (d, n) [7] and ($\alpha$, n) [8] angular distributions.

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** Supported in part by the National Science Foundation.

*Method of solution*

Using the theoretical CN formalism of Hauser and Feshbach [2], Biedenharn and Rose [3], Satchler [4], and Sheldon and Van Patter [5], augmented at option by the Moldauer modification [6], the calculation proceeds via an automatic selection and tabulation of angular momenta compatible with momentum and parity conservation restrictions, and evaluates the appropriate penetrability and Racah-function product for each combination (using subroutines for the penetrability and Racah functions). A summation of these products yields the Legendre-polynomial expansion coefficients required for the evaluation of absolute and normalized differential cross sections.

*Restrictions on the complexity of the problem*

Except that the program has been designed to cater for statistical CN formation and decay via particle (rather than $\gamma$-radiation) channels $a$, $b$ associated with known barrier penetrabilities (derived from supplementary optical-model codes) for reasonably low orbital momenta ($l \lesssim 12$), there are no inherent limitations upon the complexity of the situation considered.

*Typical running time*

A single straightforward calculation requires less than ½ minute, though this time may extend to about 30 minutes for multiple runs incorporating the Moldauer modification with relatively high orbital and spin angular momenta and with many extra exit channels.

*References*

[1] E. Sheldon and P. Gantenbein, J. Appl. Math. Phys. (ZAMP) 18 (1967) 397.
[2] W. Hauser and H. Feshbach, Phys. Rev. 87 (1952) 366.
[3] L. C. Biedenharn and M. E. Rose, Rev. Mod. Phys. 25 (1953) 729.
[4] G. R. Satchler, Phys. Rev. 94 (1954) 1304; 104 (1956) 1198; erratum in Phys. Rev. 111 (1958) 1747.
[5] E. Sheldon and D. M. Van Patter, Rev. Mod. Phys. 38 (1966) 143.
[6] P. A. Moldauer, Phys. Rev. 123 (1961) 968; 135 (1964) B642; Rev. Mod. Phys. 36 (1964) 1079.
[7] R. C. Ritter, Eric Sheldon and R. M. Strang, to be published.
[8] W. A. Schier, A. D. Robb and E. Sheldon, Bull. Am. Phys. Soc. Series II 14 (1969) 529.

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): BARBARA

*Catalogue number*: ABOB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: Burroughs B5500. *Installation*: University of Virginia, Charlottesville, Virginia, USA

*Operating system or monitor under which the program is executed*: Mark VIII

*Programming languages used*: ALGOL

*High speed store required*: 8000 words. *No. of bits in a word*: 48

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* B124 Card Reader; B321 Line Printer

*No. of cards in combined program and test deck*: 1144

*Keywords descriptive of problem and method of solution*: Nuclear, Statistical, Compound Nucleus, Mechanism, Angular Correlation, Double-Differential Cross Section, Differential Cross Section, Total Cross Section, Spin-Parity, Mixing Ratio, Multipolarity, Racah functions, Clebsch-Gordan coefficients, Racah coefficients, Fano *X*-coefficients, Legendre hyperpolynomials, Associated Legendre functions, Transmission coefficients, Optical potential, Penetrability, Spin-Orbit Coupling, Hauser-Feshbach, Moldauer, Biedenharn-Rose, Satchler.

*Nature of physical problem*

Evaluation of total and double-differential cross sections in absolute and normalized form for angular correlations in low-energy nuclear reactions of the type $(a, b\gamma)$ or $(a, b\gamma\gamma)$ according to statistical compound-nucleus theory in *j-j* coupling formalism. The program constitutes a generalization of an earlier version [1] to make provision for arbitrary spin, mass and relative orbital momentum of the interaction partners; the emergent $\gamma$-radiations may be of pure or mixed multipolarity. It can take extra exit channels and Moldauer level-width fluctuation effects into account, with provision for in-plane and/or azimuthal variation of angle.

*Method of solution*

Following automatic statistical tabulation of the relevant angular momenta, parities and summation variables permitted by conservation rules, the program evaluates Hauser-Feshbach penetrability terms [2] (with or without the Moldauer modification [3]) and Racah-function products in accordance with the compound-nucleus theory of angular correlation [4-6]. Summing the products, the code evaluates the weighting coefficients of successive orders of Legendre hyperpolynomials (bipolar spherical harmonics, expressed in terms of products of associated Legendre functions) and thence calculates the double-differential cross section in absolute and normalized form as a function of angles characterizing the emission direction of the emergent radiations.

*Restrictions on the complexity of the problem*

The program is designed to cater for *particles* of arbitrary mass, spin and orbital momentum (rather than $\gamma$-radiation) in the CN formation and decay channels, but although there is no restriction up to $l \lesssim 12$ upon the orbital momenta the computation time lengthens progressively with increase in $l_{\max}$ and in practice it is usual to restrict the partial waves to $l_{\max} \leqslant 6$. When it becomes necessary to distinguish $0^-$ from $0^+$ nuclear levels, machine-specific provisions have to be incorporated.

*Typical running time*

About 3-40 min per case, depending on the complexity, but may exceed this for high partial waves or fine angular gradation steps.

*References*

[1] E. Sheldon and P. Gantenbein, J. Appl. Math. Phys. (ZAMP) 18 (1967) 397.
[2] W. Hauser and H. Feshbach, Phys. Rev. 87 (1952) 366.
[3] P. A. Moldauer, Phys. Rev. 123 (1961) 968; 135 (1964) B642; Rev. Mod. Phys. 36 (1964) 1079.
[4] L. C. Biedenharn and M. E. Rose, Rev. Mod. Phys. 25 (1953) 729.
[5] G. R. Satchler, Phys. Rev. 94 (1954) 1304.
[6] E. Sheldon, Rev. Mod. Phys. 35 (1963) 795.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 55-63. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# NUCLEAR BOUND STATE WAVE FUNCTION SUBROUTINE

William R. SMITH
*Physics Department, Trinity University, San Antonio, Texas, USA*

Received 15 March 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): BOUND

*Catalogue number*: ACQA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/44. *Installation*: Trinity University, San Antonio, Texas, USA

*Operating system or monitor under which the program is executed*: 44PS

*Programming languages used*: FORTRAN

*High speed store required*: 60,000 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? 2540 Card Reader; 1403 Printer

*No. of cards in combined program and test deck*: 372

*Keywords descriptive of problem and method of solution*: Nuclear, Schrödinger Eqn., Wood-Saxon, Eigenfunctions, Eigenvalues, Reactions, Bound States, Wave Function, Spin-orbit, Potential, Nonlocal, Coulomb, Binding Energy, Potential Depth. Local.

*Nature of physical problem*

The subroutine BOUND numerically integrates the radial Schrödinger equation including a central Woods-Saxon potential and spin-orbit coupling for the case of a particle bound in the nuclear and Coulomb force field of a core nucleus. An important use of the subroutine itself is to provide single particle wave functions required in direct nuclear reaction calculations [1].

*Method of solution*

The requirements that the solution vanish at the origin and at infinity cause this to be an eigenvalue problem. If the number of nodes in the solution is specified, then either the binding energy or the potential depth can also be specified, and the value of the unspecified member of this pair must then be varied until it yields a solution fitting the boundary conditions. Included with the subroutine is a driver program which read parameters and print the resulting solution, energy, potential depth, number of nodes, and wave function normalization factor.

*Restrictions on the complexity of the problem*

Four options are provided: 1, 2) for a specified energy, a potential depth is 1) either provided by the user or 2) automatically estimated by the program and the program finds the nearest potential depth which satisfies the boundary conditions; 3) for a specified potential depth, an energy is provided by the user and the program finds the nearest energy which satisfies the boundary conditions; 4) for a specified energy and number of nodes, the program finds the corresponding potential depth which satisfies the boundary conditions. The potential may be either local or nonlocal. The subroutine contains 270 FORTRAN instructions and the driver program 50.

*Reference*

[1] W. Tobocman, Theory of Direct Nuclear Reactions (Oxford University Press, London, 1961).

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 67-87. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# VERSATILE PROGRAM FOR ANALYSIS OF MÖSSBAUER SPECTRA *

Michael F. BENT, Börje I. PERSSON and David G. AGRESTI
*California Institute of Technology, Pasadena, California, USA*

Received 17 July 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): MÖSSBAUER DATA LEAST-SQUARES FIT

*Catalogue number*: ABQA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/75; IBM 7094 (after minor changes). *Installation*: California Institute of Technology.

*Operating system or monitor under which the program is executed*: SYSTEM 360/OS

*Programming languages used*: FORTRAN IV (G)

*High speed store required* 40 000 words. *No. of bits in a word*: 32 binary.

*Is the program overlaid*? No (may readily be broken into 3 links if required).

*No. of magnetic tapes required*: No other than system read and write tapes.

*What other peripherals are used*? Card reader; Printer; Calcomp plotter (requires machine language control routines).

*No. of cards in combined program and test deck*: 2900.

*Keywords descriptive of problem and method of solution*: Nuclear, Solid State, Mössbauer Effect, Velocity Spectra, Hyperfine Interaction, Least-Squares Fitting, Simultaneous Fitting of Complementary Spectra.

*Nature of physical problem*
The program is designed to facilitate the analysis of experimental Mössbauer spectra in terms of hyperfine interactions.

*Method of solution*
A linearized least-squares procedure is used to adjust to the experimental data appropriate theoretical functions. An experimental spectrum is analyzed, not in terms of individual components, but rather a theoretical function is formulated using physical parameters which are adjusted in the fitting procedure. Since these parameters are usually not strongly correlated, this minimizes convergence difficulties without recourse to non-linear least-squares procedures, thereby saving computer time.

*Restrictions to the complexity of the problem*
The program may be used to fit data resulting from the overlap of source and absorber spectra, both of which may be split by hyperfine interactions. Spectra involving combined quadrupole and magnetic interaction can be analyzed if the quantization axes for the two interactions are parallel. The program can be readily adapted to most experimental situations.

*Typical running time*
On the IBM 360/75 at California Institute of Technology the loading and assembly of the program require about 30 seconds. The execution time is depending on the amount of data, the complexity of the functions to be fitted to it, and the accuracy of the initial estimates of values of parameters to be determined by the fit. To fit a function composed of 10 superimposed Lorentzians to 200 data points may require about 10 seconds of execution time.

*Unusual features of the program*
Data from complementary experiments can be simultaneously fitted in a single least-squares procedure. When data obtained under properly chosen experimental conditions are analyzed in such a combined fit, the correlations between the parameters are reduced. This increases the likelihood that the fit will converge and improve the precision in the determination of the parameters.

A wide range of physical interpretations can conveniently be tried for a given experimental spectrum, so that systematic errors can be estimated in a quantitative way.

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* This work was performed under the auspices of the U.S. Atomic Energy Commission. Prepared under Contract No. AT(04-3)-63 for the San Francisco Operations Office, U.S. Atomic Energy Commission.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 88-96. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# ASYMPTOTIC SOLUTION OF COUPLED EQUATIONS FOR ELECTRON SCATTERING

David W. NORCROSS
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Received 17 June 1969

## PROGRAM SUMMARY

*Title of program*: ASYM.

*Catalogue number*: ACQE

*Computer for which program is designed and other upon which it is operable*

*Computer*: IBM 360/65. *Installation*: University College, London.

*Operating system or monitor under which the program is executed*: SYSTEM/360

*Programming language used*: FORTRAN IV

*High speed store required*: 22 042 words. *No. of bits in a word*: 32.

*Is the program overlaid*? No.

*No. of magnetic tapes required*: None

*What other peripherals are used*? 2540 Card Reader, 1403 Printer

*No. of cards in combined program and test deck*: 1167

*Keywords descriptive of the problem and method of solution*: Atomic, Electron Scattering, Photoionization, Wave Functions, Coupled Equations, Long Range Potentials, Asymptotic Region, WBK, Threshold.

*Nature of physical problem*

The program ASYM solves coupled second-order differential equations of the type encountered in the close-coupling formulation of electron-atom (ion) scattering problems, at some specified point in the asymptotic region. Lineraly independent sets of wave functions are found which could be used as boundary solutions for a complete solution of the close-coupling integro-differential equations [1].

*Method of solution*

For a particular reaction channel and associated boundary condition, the program uses the more appropriate of two methods fcr determining the asymptotic solutions. One method, which involves assuming the asymptotic form for the phase of the solution and solving for the amplitude by an asymptotic series expansion, is well known and widely used [2]. The second method, which involves assuming the first order WBK solution for the phase [3] and interating on the amplitude, is new and was designed to replace the first in regions where it fails. Asymptotic solutions can now be obtained for the equations representing scattering near thresholds, or from highly ionized atoms.

*Restrictions on the complexity of the program*

The program is designed to work for scattering from neutral atoms or positive ions, with at least one reaction channel open. It will cope with any number of channels up through six, and long range potentials up through $r^{-5}$. These limitations on the capacity of the program can be increased easily by the user if required.

*Typical running time*

The "worst case" running time is of the order of $1.5 \times N^2$ seconds, where $N$ is the number of reaction channels, and compilation time is about 45 seconds. These figures are for the IBM 360/65 at University College. When some channels are closed or there are no near-threshold channels running time is greatly reduced.

*References*

[1] D. W. Norcross and M. J. Seaton, J. Phys. B (Proc. Phys. Soc.) [2] 2 (196) 731.
[2] P. G. Burke and H. M. Shey, Phys. Rev. 126 (1962) 147.
[3] D. R. Burgess, Proc. Phys. Soc. 81 (1963) 442.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 97-105. NORTH-HOLLAND PUBLISHING COMP.. AMSTERDAM

# A PROGRAM FOR CALCULATING REGGE TRAJECTORIES IN POTENTIAL SCATTERING

P. G. BURKE
*Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast, Northern Ireland*

and

C. TATE
*Department of Physics, University of York, York, UK*

Received 11 July 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): Regge Trajectory

*Catalogue number*: AAGA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: I.C.L. 1907. *Installation*: The Queen's University of Belfast.

*Operating system or monitor under which the program is executed*: Q.U.B. operating system.

*Programming languages used*: FORTRAN IV

*High speed store required*: 10624 words. *No. of bits in a word*: 24

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1187

*Keywords descriptive of problem and method of solution*: Schrödinger, $S$-matrix, Nuclear, Phase-shift, Scattering, Bound-state, Pole, Regge, Complex, Angular momentum, Gamma function, Bessel function, Yukawa Potential, Eigenvalue, Trajectory.

*Nature of the physical problem*

This program solves the radial Schrödinger equation and finds the positions and residues of Regge poles [1] for a Yukawa potential and follows these poles automatically as a function of energy. Alternatively, it will compute the $S$-matrix and phase shifts at a specified grid of points in the complex angular momentum plane and for a given set of energies. The program can be modified to calculate Regge trajectories for any potential which can be specified by an analytic formula.

*Method of solution*

The radial Schrödinger equation is integrated numerically inwards and outwards using the Runge-Kutta-Gill method. The $S$-matrix is determined by fitting the solution to a complex Bessel function, and the poles in the $S$-matrix are found by Newton's iteration method.

*Restrictions on the complexity of the program*

The program is limited to real positive and negative values of the energy and to all complex angular momenta except the half odd integers.

*Typical running time*

The evaluation of the $S$-matrix at one point takes about six seconds on the I.C.L. 1907. To determine the position of a pole in the $S$-matrix takes about 40 seconds for a typical number of iterations.

*References*

[1] T. Regge, Nuovo Cimento 14 (1959) 951; 18 (1960) 947.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 106-112. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# NUCLEAR PENETRABILITY AND PHASE SHIFT SUBROUTINE

William R. SMITH
*Physics Department, Trinity University, San Antonio, Texas, USA*

Received 16 July 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): SCAT

*Catalogue number*: ACQF

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600; IBM 360/44. *Installation*: The University of Texas, Austin, Texas, USA
Trinity University, San Antonio, Texas, USA

*Operating system or monitor under which the program is executed*: Scope 2.0 highly modified

*Programming languages used*: Fortran.

*High speed store required*: 20.000 words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? None

*No. of cards in combined program and test deck*: 340

*Keywords descriptive of problem and method of solution*: Nuclear, Schrödinger eq., Woods-Saxon, Spin-orbit, Potential, Nonlocal, Coulomb, Reflection factors, Penetrabilities, Transmission Coefficients, Phase Shifts, Scattering, Optical model.

*Nature of physical problem*
The subroutine SCAT numerically integrates the radial Schrödinger equation including a complex central Woods-Saxon potential and spin-orbit coupling for the case of a particle scattered by the nuclear and Coulomb force field of a target nucleus. The subroutine provides penetrabilities needed in the treatment of compound nucleus reactions [1] and also phase shifts necessary to calculate elastic scattering and polarization angular distributions and reaction, total elastic and total cross sections.

*Method of solution*
Starting at the origin, the solution is generated out to two points beyond the nuclear potential where the solution is matched to a linear combination of regular and irregular Coulomb wave functions. The penetrabilities and phase shifts are derived from the coefficients in this linear combination.

*Restrictions on the complexity of the problem*
The maximum number of partial waves is 31 and the maximum projectile spin is 1, but both of these numbers can be easily changed by altering the storage allotted to certain variables. The spin-orbit potential is a function of the derivative of the real part of the central potential and is real; however, the imaginary part of the central potential is independent of the real part, and may be any mixture of volume and surface-peaked forms.

*Typical running time*
The test case requires 2.5 seconds to compile and 0.2 seconds to run on the CDC 6600 computer at the University of Texas.

*Unusual features of the program*
The central potential may be either local or nonlocal, the latter option being treated by means of the local energy approximation [2].

*References*

[1] W. Hauser and H. Feshbach, Phys. Rev. 87 (1952) 366.
[2] F. G. Perey and D. S. Saxon, Phys. Letters 10 (1964) 107.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 113-134. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# RELATIVISTIC AND NON-RELATIVISTIC CONFIGURATION INTERACTION CALCULATIONS FOR ATOMS HAVING A CLOSED CORE AND TWO VALENCE SPIN-ORBITALS *

Donald R. BECK and Richard N. ZARE
*Joint Institute for Laboratory Astrophysics* ‡
*University of Colorado, Boulder, Colorado, USA*

Received 2 July 1969

## PROGRAM SUMMARY

*Title of program*: SOCKITTOME 1

*Catalogue number*: AAKA

*Computer for which the program is designed and others upon which it is operable*:

*Computer*: CDC 6400. *Installation*: University of Colorado

*Operating system or monitor under which the program is executed*: 6400/6500/6600 Scope Version 3.1.3

*Programming languages used*: FORTRAN IV

*High speed store required*: 141 $000_8$ words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 3243

*Keywords descriptive of problem and method of solution*: Central Field Approximation, Configuration Interaction, Low-$Z$ Pauli Approximation, Modified Hartree-Fock-Slater Equation, Linear Variation Technique, Self-Consistent Field.

*Nature of physical problem*

The problem is to obtain [1,2] wavefunctions for bound atomic levels which permit accurate calculation of energies and transition probabilities. The low-$Z$ Pauli approximation [3], which is correct to orders $Z^3\alpha^2$ and $Z^4\alpha^2$ in the energy (the non-relativistic energy is of order $Z^2$) is used to approximate the atomic Hamiltonian. The anti-Hermitian part of those operators characteristic of the Dirac theory is dropped.

*Method of solution*

The wavefunction is expanded in single configuration functions which are eigenstates of $S^2$, $L^2$, $J^2$, $J_z$, and parity. All configurations in the expansion must have a closed core and two valence spin-orbitals. The single configuration functions are a linear combination of Slater determinants whose elements are of the central field type. The radial part of the elements is obtained from Lindgren's [4] modification of the Hartree-Fock-Slater [5] equation which is solved using the methods of Herman and Skillman [6]. (Three subprograms were originally written by Herman and Skillman in Fortran II. All statements incompatible with Fortran IV as defined in the Control Data 6400/6500/6600 Computer Systems Manual were altered so as to be compatible with Fortran IV.) The coefficients are obtained by application of the variational principle (linear variation technique). The program allows exclusion of any relativistic operators and consequently strictly non-relativistic calculations may also be done.

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* Supported by Atomic Energy Commission Contract AT(30-1)-3408, and by the Advanced Research Projects Agency of Department of Defense monitored by Army Research Office-Durham under Contract No. DA-31-124-ARO-D-139.

‡ of the National Bureau of Standards and the University of Colorado.

### *Restrictions on the complexity of the problem*

The program requires $141\,000_8$ high speed core locations at 60 bits per word. The 32 bits per word of the IBM 360 may not suffice.

### *Typical running time*

The running time (all operators) for a test case (Ba I with the $6s^2$, $6s7s$, $6p^2(^1S_0, ^3P_0)$, $6p7p$, $5d^2$, $5d6d$ configurations for even parity and $J = 0$) was six minutes on the CDC 6400. A more realistic expansion (one containing 25-30 terms) would take about one hour of CDC 6400 computing time.

### *References*

[1] R. N. Zare, J. Chem. Phys. 45 (1966) 1966; 47 (1967) 3561; JILA Report No. 80 (1966), unpublished; E. Trefftz and R. N. Zare, J. Quant. Spectry. Radiative Transfer 9 (1969) 643.

[2] D. R. Beck, J. Chem. Phys., accepted for publication (Sept., 1969); Ph. D. thesis, Lehigh University (1968), unpublished.

[3] H. A. Bethe and E. E. Salpeter, Quantum mechanics of one- and two-electron atoms (Academic Press, New York, 1957) p. 181.

[4] E. R. Cohen and J. W. M. DuMond, Rev. Mod. Phys. 37 (1965) 537.

[5] E. U. Condon and G. H. Shortley, The theory of atomic spectra (Cambridge Univ. Press, New York, 1935).

[6] A. R. Edmonds, Angular momentum in quantum mechanics (Princeton Univ. Press, Princeton, 1960).

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 135-140. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# PARAMETER SEARCH SUBROUTINE

William R. SMITH
*Physics Department, Trinity University, San Antonio, Texas, USA*

Received 4 June 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): SEARCH

*Catalogue number*: ABOD

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/44. *Installation*: Trinity University, San Antonio, Texas, USA

*Operating system or monitor under which the program is executed*: 44PS

*Programming languages used*: FORTRAN

*High speed store required*: 550 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? 2540 Card Reader; 1403 Printer

*No. of cards in combined program and test deck*: 202

*Keywords descriptive of problem and method of solution*: Parameter Optimization, Least-Squares, Root-Mean-Square Minimization, Curve Fitting.

*Nature of physical problem*

Many computational problems require several parameters to be adjusted so that agreement with certain data is obtained. The subroutine SEARCH does this job automatically and can be adapted for used with any program with a minimum of difficulty.

*Method of solution*

The subroutine finds for each parameter the parameter value which causes the derivative, with respect to the parameter, of the root-mean-square deviation between data and calculation to vanish. Employing the method developed by Maddison [1], this minimization is carried out by means of a first order Taylor series expansion of the calculated results about some initial set of parameter values and replacement of derivatives at the minimizing parameter values with derivatives at the initial parameter values. The result is a set of simultaneous equations to be solved for the differences between the initial parameter values and the best-fit parameter values. If the predicted shift in any parameter is greater than 10%, then a step-wise search along the predicted parameter gradient is performed.

*Restrictions on the complexity of the problem*

As set up, a maximum of 20 parameters and 200 data points can be simultaneously treated. However, these numbers can be arbitrarily increased or decreased by changing the dimensions of variables, so that the size restrictions essentially depend only on the computer storage available.

*Typical running time*

The test case requires 88 seconds to compile and 6 seconds to run on the IBM 360 computer at Trinity University.

*Reference*

[1] R.N. Maddison, Proc. Phys. Soc. (London) 79 (1962) 264.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 151-166. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# A MULTI-CONFIGURATION HARTREE–FOCK PROGRAM

Charlotte FROESE FISCHER
*Department of Applied Analysis and Computer Science,*
*Faculty of Mathematics, University of Waterloo, Waterloo, Ontario, Canada*

Received 19 November 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): MULTI-CONFIGURATION HARTREE–FOCK

*Catalogue number*: ACQJ

*Computer for which the program is designed and others upon which it is operable*

*Computer*: S360/75. *Installation*: University of Waterloo

*Operating system or monitor under which the program is executed*: OS/360 - MVT and HASP II

*Programming languages used*: FORTRAN IV

*High speed store required*: 180k bytes. *No. of bits in a byte*: 8

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader, Punch, Printer

*No. of cards in combined program and test deck*: 1972

*Keywords descriptive of problem and method of solution*: Atomic Structure, Numerical Hartree–Fock, Configuration Interaction, Bound State, Schrödinger Equation, Wave Function, Self-Consistent Field. Energy Level.

*Nature of physical problem*

Numerical non-relativistic Hartree–Fock results are determined within the multi-configuration approximation for atoms in a bound state.

*Method of solution*

The self-consistent field method of solution is employed.

The orthogonality conditions

$$\int P(nl;r)\,P(n'l;r)\,\mathrm{d}r = \delta_{nn'}\,,$$

are applied only to functions within a configuration. These conditions lead to off-diagonal energy parameters in the Hartree–Fock equations. When two incomplete groups with the same occupation number and the same angular quantum number $l$ are present, the off-diagonal energy parameters are assumed to be zero which will not always lead to orthogonal wave functions [1].

*Restrictions on the complexity of the problem*

The possible configurations are restricted to those for which the interactions can be expressed as either $F^k$, $G^k$, or $R^k$ integrals. This excludes certain singly substituted configurations which frequently would result in an indeterminate system of equations, [2]. Also, since bound states in the continuum interact most strongly with continuum states, a multi-configuration calculation for such states cannot be performed with this program.

*Unusual features of the program*

The organization of the program is such that the "frozen core" approximation may be used and orbitals with zero occupation number are allowed.

*Typical running time*

The CPU time for a series of cases consisting of
(i) the two-configuration approximation for $C^{2+}$, $B^{+}$ and Be $^1S$
(ii) Na 3p $^2P$
(iii) Na 3s $^2S$ with 1s, 2s, 2p "frozen"
(iv) Na 4s $^2S$ with 1s, 2s, 2p "frozen" and the 3s having a zero occupation number
required 1.48 min on an IBM 360/75.

*References*

[1] C. Froese, Can. J. Phys. 45 (1967) 7.
[2] C. Froese Fischer, J. Phys. B, submitted for publication.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 167-180. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# COMPUTATION OF WAVEFUNCTIONS FOR THE HELIUM ISOELECTRONIC SEQUENCE

H. O. KNOX
*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, Northern Ireland*

Received 20 November 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): TWO-ELECTRON WAVEFUNCTIONS

*Catalogue number*: ACQK

*Computer for which the program is designed and others upon which is it operable*

*Computer*: ICL 1907. *Installation*: Queen's University of Belfast

*Operating system or monitor under which the program is executed*: QUBE

*Programming languages used*: FORTRAN

*High speed store required*: 20.000 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: One may be used to store the results

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1754

*Keywords descriptive of problem and method of solution*: Atomic Wavefunctions, Helium Isoelectronic Sequence, Sturmian Functions, Configuration Interaction, Inverse Iteration, Eigenvalues, Bound State, Schrödinger Equation, Autoionizing State, Resonance Energy, Energy Level

*Nature of the physical problem*

This program computes wavefunctions and energies of the helium isoelectronic sequence to any desired accuracy. The wavefunctions have the correct asymptotic form and therefore they are particularly suitable for use in scattering problems. They have been used to calculate line strengths by Knox and Rudge [1].

*Method of solution*

The wavefunction is of the configuration interaction type

$$\Psi = \mathcal{A}\chi(SM_S,\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2) \sum_{n_1 n_2} \sum_{i} a(n_1 n_2 i)\, y(l_1 l_2 L|\hat{\boldsymbol{r}}_1 \hat{\boldsymbol{r}}_2) \frac{1}{r_1 r_2} F_{n_1 l_1}(\alpha_1 r_1) F_{n_2 l_2}(\alpha_2 r_2) .$$

where $\mathcal{A}$ is the anti-symmetrizing operator, $\chi$ is the two-electron spin function, $i$ represents the orbital angular momenta quantum numbers $(l_1 l_2 L)$ and $F_{nl}(\alpha r)$ is a Sturmian function. The matrix formulation of the variational principle is used, the energy closest to the experimental energy and the corresponding wavefunction being extracted using an inverse powering method described by Wilkinson [2].

*Restrictions on the complexity of the problem*

The size of the wavefunction is limited by the storage available and by rounding errors in the calculation of the matrix elements and in matrix inversion. The major storage requirement is for four matrices whose dimension equals the number of basis functions used; the matrix elements become inaccurate if $n_1, n_2 > 10$; and it is not recommended that the present matrix inversion routine be used on matrices larger than 60 × 60.

*Typical running time*

The time required to compute one energy and wavefunction increases roughly as $N^2$ where $N$ is the number of basis functions used and for $N = 10$ it is about 22 seconds on an ICL 1907. The time needed for different wavefunctions of the same size may vary considerably due to the use of an iterative routine.

*References*

[1] H. O. Knox and M. R. H. Rudge, J. Phys. B (Ser. 2) 2 (1969) 521.
[2] J. H. Wilkinson, The algebraic eigenvalue problem (Clarendon Press, Oxford, 1965).

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 181-190. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# HAUSER-FESHBACH NUCLEAR SCATTERING SUBROUTINE LIANA

William R. SMITH
*Physics Department, Trinity University, San Antonio, Texas, USA*

Received 22 October 1969

## ADAPTATION SUMMARY

*Title of manuscript*: Adaptation of Subroutine SCAT for Use with Program LIANA

*Adaptors' names and addresses*: William R. Smith, Physics Department, Trinity University, San Antonio, Texas, USA

*Title of adaptation* (32 characters maximum): ADAPT SCAT TO LIANA

*Adaptation number*: 0002

*Reference to original program*: *Catalogue number*: ACQF; *Title*: SCAT; *Ref. in CPC*: 1 (1969) 106

*Authors of original program*: William R. Smith

*No. of cards required to effect adaptation* (including directive cards): 13

## PROGRAM SUMMARY

*Title of manuscript*: Hauser-Feshbach Nuclear Scattering Subroutine LIANA

*Authors' names and addresses*: William R. Smith, Physics Department, Trinity University, San Antonio, Texas, USA

*Title of program* (32 characters maximum): LIANA

*Catalogue number*: ABKA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6400, CDC 6600. *Installation*: Computer Knowledge Corporation, San Antonio, Texas; resp. University of Texas, Austin, Texas, USA

*Operation system or monitor under which the program is executed*: SCOPE 3.1.6A

*Programming language used*: FORTRAN

*High speed store required*: 23,000 words. *No. of bits per word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? None

*No. of cards in combined program and test deck*: 571

*CPC Library subprograms used*

*Catalogue number*: ACQF; *Title*: SCAT; *Ref. in CPC*: 1 (1969) 106

*Adaptation number*: 0002; *Adaptation title*: ADAPT SCAT TO LIANA; *Ref. in CPC*: 1 (1969) 181.

*Keywords descriptive of problem and method of solution*: Nuclear, Reaction, Compound Nucleus, Compound-Elastic, Hauser–Feshbach, Differential Cross Section, Integrated Cross Section, Optical Model, Woods–Saxon, Spin-Orbit, Penetrabilities, Width Fluctuation Correction.

*Nature of physical problem*

Subroutine LIANA computes the scattering angular distribution and integrated cross section for any two-particle nuclear reaction which proceeds through a statistical distribution of compound nucleus states. The subroutine may be incorporated into other programs or else run with the driver program provided. The latter calls subroutine SCAT [1] to obtain the necessary optical model nuclear penetrabilities. The input required consists of the energies, charges, masses, spins, parities, and optical model parameters for all two-particle channels through which the compound nucleus can decay.

*Method of solution*

The Hauser–Feshbach theory [2] generalized [3] to include spin-orbit coupling is employed. Either the plain Hauser–Feshbach method implying independence of compound nucleus formation and decay or the modified Hauser–Feshbach procedure including a correction [4] for an assumed Porter–Thomas distribution of compound nucleus resonance widths [5] may be utilized.

*Restrictions on the complexity of the problem*

Only particle channels can be treated; gamma-ray channels are excluded. Nor can channels containing three or more separate particles be handled. In any channel the spin-orbit particle can have spin up to 5 and the other particle may have any spin. The maximum number of partial waves necessary in any one channel can be no greater than 31. A total of ten types of two particle partitions, and a total of 600 channels, may be simultaneously treated. The restrictions on maximum spin, number of partial waves, number of particle types, and number of channels are due solely to storage allotments and may be easily relaxed.

*Typical running time*

The running time is roughly proportional to the number of penetrabilities calculated, since the rest of the calculation is short by comparison. The calculational time spent by LIANA alone increases as the values of the spin, number of channels, and number of partial waves increase. The test case requires 13 seconds to compile and 3 seconds to run on a CDC 6400 computer.

*References*

[1] W. R. Smith, Computer Phys. Commun. 1 (1969) 106.

[2] W. Hauser and H. Feshbach, Phys. Rev. 87 (1952) 366.

[3] G. R. Satchler, Proc. Phys. Soc. (London) A68 (1955) 1041.

[4] P. Moldauer, Phys. Rev. 123 (1961) 968.

[5] C. E. Porter and R. G. Thomas, Phys. Rev. 104 (1956) 483.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 191-197. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# VECTOR COUPLING COEFFICIENTS FOR COMPLEX ATOMS

H. NUSSBAUMER *
*Department of Physics, University College London, London, UK*

Received 30 September 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): VECTOR COUPLING COEFFICIENTS

*Catalogue number*: ACQH

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/65. *Installation*: University College London

*Operating system or monitor under which the program is executed*: System/360

*Programming languages used*: FORTRAN IV

*High speed store required*: 15,300 words. *No. of bits in a word*: 32

*Is the program overlaid*? Yes

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader, Line Printer, Magnetic Disk is optional

*No. of cards in combined program and test deck*: 1634

*Keywords descriptive of problam and method of solution*: Atomic, Complex atoms, Wave function, Slater states Bound states, *LS* coupling, Configuration

*Nature of physical problem*

The program calculates vector coupling coefficients and Slater determinants to represent the eigenfunctions of a complex atom in the one-configuration representation as a linear combination of Slater states. It works in the *L-S* coupling scheme. It allows for *SL* degeneracy.

*Method of solution*

The coupling coefficients for those functions with $M_L = 0$ and $M_S = 0$ or $\frac{1}{2}$ are calculated by direct diagonalisation of the operators $L^2$ and $S^2$. The other coefficients are obtained by applying the step-up or step-down operators. The phase relation is the one adopted by Condon and Shortley [1]. The orthonormality of the functions is checked for accuracy in 13 figures.

The input consists of a list of the principal quantum numbers of the $N$ electrons in the configuration to be treated and information about whether to store the results on disk. The output consists of the term list, the Slater determinants, and the vector coupling coefficients.

*Restrictions on the complexity of the problem*

The published version accepts up to seven electrons. This and other limits imposed by the high speed core and listed in the LONG WRITE-UP can easily be changed.

*Typical running time*

The complete program requires 90 sec for compilation and linkage.

*Reference*

[1] E. U. Condon and G. H. Shortley, The theory of atomic spectra (Cambridge University Press, London, 1935).

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* Present address: Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado 80302, USA.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 198-206. NORTH-HOLLAND PUBLISHING COMP.. AMSTERDAM

# NUCLEAR ELASTIC SCATTERING PROGRAM WITH PARAMETER SEARCH

William R. SMITH
*Physics Department, Trinity University, San Antonio, Texas, USA*

Received 20 August 1969

## ADAPTATION SUMMARY

*Title of manuscript*: Adaptation of Subroutine SCAT for Use with Program ELASTIC

*Adaptor's names and addresses*: William R. Smith, Physics Department. Trinity University. San Antonio, Texas, USA

*Title of adaptation* (32 characters maximum): ADAPT SCAT TO ELASTIC

*Adaptation number*: 0001

*Reference to original program*: *Catalogue number*: ACQF; *Title*: SCAT; *Ref. in CPC*: 1 (1969) 106

*Authors of original program*: William R. Smith

*No. of cards required to effect adaptation* (including directive cards): 12

## ADAPTATION SUMMARY

*Title of manuscript*: Adaptation of Subroutine SEARCH for Use with Program ELASTIC

*Adaptor's names and addresses*: William R. Smith, Physics Department, Trinity University. San Antonio, Texas, USA

*Title of adaptation* (32 characters maximum): ADAPT SEARCH TO ELASTIC

*Adaptation number*: 0001

*Reference to original program*: *Catalogue number*: ABOD; *Title*: SEARCH; *Ref. in CPC*: 1 (1969) 135

*Authors of original program*: William R. Smith

*No. of cards required to effect adaptation* (including directive cards): 2

## PROGRAM SUMMARY

*Title of manuscript*: Nuclear Elastic Scattering Program with Parameter Search

*Author's names and addresses*: William R. Smith. Physics Department. Trinity University. San Antonio, Texas, USA

*Title of program* (32 characters maximum): ELASTIC

*Catalogue number*: ACQG

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: University of Texas, Austin. Texas. USA

*Operating system or monitor under which the program is executed*: Scope 2.0 Highly Modified

*Programming languages used*: FORTRAN

*High speed store required* 25,000 words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*No. of cards in combined program and test deck*: 290

*CPC Library subprograms used*

*Catalogue number*: ABOD; *Title*: SEARCH; *Ref. in CPC*: 1 (1969) 135

*Adaptation number*: 0001; *Adaptation title*: ADAPT SEARCH TO ELASTIC: *Ref. in CPC*: 1 (1969) 198.

*Catalogue number*: ACQF: *Title*: SCAT; *Ref. in CPC*: 1 (1969) 106

*Adaptation number*: 0001; *Adaptation title*: ADAPT SCAT TO ELASTIC: *Ref. in CPC*: 1 (1969) 198.

*Keywords descriptive of problem and method of solution*: Nuclear. Elastic scattering. Spin-orbit. Coulomb. Woods-Saxon. Potential. Local. Nonlocal. Optical model.

*Nature of physical problem*

Program ELASTIC optimizes the parameters of a nuclear optical model potential including spin-orbit coupling and calculates the angular distribution of the corresponding elastic scattering cross section [1].

*Method of solution*

Legendre polynomials and Coulomb phase shifts are calculated by recursion, nuclear phase shifts are obtained with subroutine SCAT [2], and the cross sections are then calculated at specified angles by summing over partial waves. Subroutine SEARCH [3] is employed to optimize the parameters of the optical model potential.

*Restrictions on the complexity of the problem*

The program is applicable to any projectile, but only projectiles with spin $\frac{1}{2}$ or 1 can be treated with spin-orbit coupling. The Coulomb potential corresponds to a homogeneously charged sphere, the spin-orbit potential is real and its parameters are the same as those for the real part of the central potential, and the maximum number of partial waves is 31, although this number can be easily increased.

*Typical running time*

The running time depends greatly on the nature of the parameter search. The test case, which includes a 3-cycle search on two parameters, requires 4.6 seconds to compile and 1.4 seconds to run on the CDC 6600 computer at The University of Texas.

*Unusual features of the program*

The central potential may be either local or approximately nonlocal.

*References*

[1] A. Messiah, Quantum mechanics, Vol. 1 (North-Holland, Amsterdam, 1958).

[2] W. R. Smith, Computer Phys. Commun. 1 (1969) 106.

[3] W. R. Smith, Computer Phys. Commun. 1 (1969) 135.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 207-215. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# ARBITRARY $3n$-$j$ SYMBOLS FOR SU(2) *

JOEL SHAPIRO
*Department of Physics, University of California,*
*Berkeley, California, USA*

Received 30 October 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): $3n$-$j$ SYMBOLS FOR SU(2)

*Catalogue number*: AAYA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: Lawrence Radiation Laboratory, Berkeley

*Operating system or monitor under which the program is executed*: BKY 37

*Programming languages used*: CDC EXTENDED FORTRAN

*High speed store required*: 14,000 words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Disc

*No. of cards in combined program and test deck*: 844

*Keywords descriptive of problem and method of solution*: Nuclear, Atomic, Nuclear Spectra, Nuclear Structure, Atomic Spectra, Atomic Structure, Angular Momentum, Matrix Element, Crossing Matrices, Transformation Matrices, Recoupling Coefficient, Racah Coefficient, Wigner Coefficient, Fano Coefficient, 3-$j$, 6-$j$, 9-$j$, 12-$j$, 15-$j$, 18-$j$, 21-$j$, $3n$-$j$ Symbols, Representation of Three Dimensional Rotation Group.

*Nature of physical problem*

An arbitrary $3n$-$j$, or recoupling, coefficient can be represented by a diagram *** consisting of $2n$ vertices connected by $3n$ directed line segments, with three lines connected to each vertex. This Fortran program will write a Fortran function to evaluate a given arbitrary $3n$-$j$ coefficient.

*Method of solution*

Triangles within the diagram are eliminated by multiplying by a 6-$j$ symbol. If no triangles exist, the polynomial with the smallest number of sides is reduced, one side at a time, by multiplying by a 6-$j$ symbol and summing over one angular momentum. In the end, the symbol is reduced to a sum of products of 6-$j$ symbols.

*Restrictions*

The current program will work for $n \leqslant 20$. Adjustments for larger $n$ are discussed in the long write-up. The output function must be used together with a 6-$j$ function. The present 6-$j$ routine requires the sum of four of the angular momenta to be $< 100$.

*Unusual features of the program*

The compilation and execution of the program is in two sections. The first part of the deck is read in, compiled and executed, causing the generation of Fortran Function subprograms defining $3n$-$j$ symbols as specified by data cards. The rest of the subroutines are then read in and compiled together with the newly generated Functions. More data is then read and the values of the $3n$-$j$ symbols are calculated.

*Reference*

[1] A. P. Yutsis, I. B. Levinson and V. V. Vanagas, The theory of angular momentum (Oldbourne Press, London, 1962).

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* This work was supported in part by the U.S. Atomic Energy Commission.

*** The graphical representation of the $3n$-$j$ symbol used is due to Yutsis et al. [1].

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 216-222. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

# HARTREE FOCK SLATER SELF CONSISTENT FIELD CALCULATIONS

J. P. DESCLAUX

*Commissariat à l'Energie Atomique, C.E.L., B.P. 27, 94 Villeneuve-St-Georges, France*

Received 23 September 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): H.F.S. SELF CONSISTENT FIELD

*Catalogue number*: ACQI

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/50. *Installation*: C.E.L., B.P. n$^{o}$. 27, 94-Villeneuve-St-Georges, France

*Operating system or monitor under which the program is executed*: O S MFT 2

*Programming languages used*: FORTRAN

*High speed store required*: 22160 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? 2540 Card Reader; 2540 Card Punch; 1403 Printer

*No. of cards in combined program and test deck*: 635

*Keywords descriptive of problem and method of solution*: Atomic, Hartree Fock equations, Free electron exchange potential, Eigenfunctions, Eigenvalues, Numerov Method, Pratt improvement scheme.

### *Nature of the physical problem*

With present programs the Hartree-Fock (H.F.) equations can be treated for nearly all configurations. It has been shown [1], however, that accurate electron binding energies can be obtained without use of the comparatively complicated H.F. scheme. Since the main difficulty posed by the H.F. equations is the treatment of the non local exchange potential it would be desirable to find a good local approximation to the H.F. potential. The approximation suggested by Slater [2] is used in this program as it has been in many atomic or energy band calculations.

### *Method of solution*

The H.F. equations are solved by the "IN-OUT" method described by Hartree [3]. The numerical procedure is that of Numerov with the "tail procedure" introduced by Froese [4]. The improvement scheme of Pratt, as described in [1] page 4-8, is used to accelerate the convergence.

### *Restrictions on the complexity of the problem*

In the present work single electronic configurations having one or more open shells are treated on the same basis as closed shells configurations. The distinctive features introduced by the presence of unmatched spins are not considered. The electronic configuration is specified by the orbital occupation numbers only. The program is restricted to free atoms or positive ions and the maximum number of one electron orbitals is 20.

### *Typical running time*

The test case (neutral mercury atom) requires 110 seconds to compile and 151 seconds to run on the IBM 360/50 computer. The starting potential being the Thomas Fermi potential for the free atom, an analytical approximation of which is included in the program.

### *References*

[1] F.Herman and S.Skillman, Atomic structure calculations (Prentice Hall, Englewood Cliffs, New Jersey, 1963).
[2] J.C.Slater, Phys. Rev. 81 (1951) 385.
[3] D.R.Hartree, The calculation of atomic structure (John Wiley, New York, 1957).
[4] Ch.Froese, Can. J. Phys. 41 (1963) 1895.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 223. NORTH-HOLLAND PUBLISHING COMP., AMSTERDAM

## ERRATUM NOTICE

*Title of manuscript*: A program to calculate Franck–Condon factors
*Author*: A. C. Allison
*Reference*: Computer Physics Communications 1 (1969) 21.
*Title of program*: FRANCK- CONDON FACTOR PROGRAM
*Catalogue number*: AACA

## ERRATUM

E. Sheldon and R. M. Strang, Computation of total, differential, and double-differential cross sections for compound nuclear reactions of the type (a, b), (a, b$\gamma$) and (a, b$\gamma$-$\gamma$) (II) Generalized programs "MANDY" and "BARBARA" for arbitrary angular momenta in Hauser–Feshbach–Moldauer formalism, Computer Physics Communications 1 (1969) p. 35.

In a definition featured half-way down the left-hand column of p. 49,

CØNST = 51.849 08 $\hat{=}\ \bar{\lambda}^2 E_1/4\pi$,

should read

CØNST = 52.250 75 $\hat{=}\ \bar{\lambda}^2 E_1 m_i/4$.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 225-231. NORTH-HOLLAND PUBLISHING COMPANY

# COEFFICIENTS OF FRACTIONAL PARENTAGE IN $j-j$ COUPLING IN THE ISOSPIN REPRESENTATION

Lincoln B. HUBBARD
*Oak Ridge National Laboratory, Oak Ridge, Tennessee*
*and*
*Knoxville College, Knoxville, Tennessee*

Received 3 March 1970

## PROGRAM SUMMARY

*Title of program*: JJTCFP

*Catalogue number*: ABKB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM-360/75 and 91. *Installation*: Oak Ridge National Laboratory, Oak Ridge, Tennessee. USA.

*Operating system or monitor under which the program is executed*: OS360

*Programming languages used*: FORTRAN IV (H)

*High speed store required*: 43 500 words. *No. of bits in word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Standard card-reader punch and printer

*No. of cards in combined program and test deck*: 714

*Keywords descriptive of problem and method of solution*: Nuclear, cfp, fpc, Angular Momentum, Wave Functions, Shell Model, $j-j$ Coupling.

*Nature of physical problem*

The program JJTCFP evaluates the coefficients of fractional parentage [1, 2], c.f.p., in the $j-j$ coupling scheme for eigenstates of seniority, $i$-spin and total angular momentum. This program is applicable to any shell and can be used for fermions of only one type such as electrons.

*Method of solution*

The program JJTCFP uses a recursion relation [3] to find the $n$-($n$+1) c.f.p. from a table of ($n$-1)-$n$ c.f.p. As a result, the program is not suitable as a subroutine, but could be used in an overlaid configuration.

*Restrictions on the complexity of the problem*

This program is directly applicable to any $j-j$ shell in the $i$-spin formalism or in maximum $i$-spin only. However, the dimension of the arrays must be increased if the program is to be used near the center of the shells for shells having $j \geqslant 7/2$.

*Typical running time*

The sample output required less than one second on the IBM-360/91; compile time is a few seconds. The $j = 7/2$ 4-5 c.f.p. table (nearly 10 000 c.f.p., about half of which were zero) required 2 minutes of execution on the same machine.

*Unusual features of the program*

External sorting of output from one stage is required before it is used as input to the next stage.

*References*

[1] R. F. Bacher and S. Goudsmit, Phys. Rev. 63 (1934) 948.
[2] G. Racah, Phys. Rev. 63 (1943) 367.
[3] A. Deshalit and I. Talmi, Nuclear shell theory (Academic Press, New York, 1963).

* Research sponsored by the U.S. Atomic Energy Commission in part under contract with the Union Carbide Corporation and in part under contract AT(30-1)-2098.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 232-240. NORTH-HOLLAND PUBLISHING COMPANY

# COLLISION STRENGTHS FROM REACTANCE MATRICES

H. E. SARAPH
*Physics Department, University College, London W.C. 1, UK*

Received 4 December 1969

## PROGRAM SUMMARY

*Title of program*: (32 characters maximum): SIMMEG

*Catalogue number*: AAGB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/65; CDC 60 version. *Installation*: UCL London

*Operating system or monitor under which the program is executed*: OS/360

*Programming languages used*: FORTRAN IV

*High speed store required*: 4187 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? None

*No. of cards in combined program and test deck*: 698

*Keywords descriptive of problem and method of solution*: Atomic Scattering, Reactance Matrix, Inelastic Collision Cross Section, *LS* Coupling, Total Cross Section.

*Nature of physical problem*

A standard format for the storage of reactance matrices is proposed. Collision cross sections are computed from these data.

*Method of solution*

The data are sorted and checked for completeness. The computation proper uses matrix algebra.

*Restrictions on the complexity of the problem*

The lengths of the arrays may be adjusted to suit the problem and the store available in the computer.

*Typical running time*

Compile time 1 min, execution of sample data, 175 cards, 9 sec.

*Unusual features of the program*

Double length, 8 bytes per word, is used for most variables.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 241-250. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM TO CALCULATE A GENERAL RECOUPLING COEFFICIENT

P. G. BURKE

*School of Physics and Applied Mathematics, The Queen's University of Belfast, Belfast, Northern Ireland*

Received 21 January 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): NJSYM

*Catalogue number*: AAGD

*Computer for which the program is designed and others upon which it is operable*

*Computer*: I.C.L. 1907. *Installation*: Queen's University, Belfast

*Operating system or monitor under which the program is executed*: Q.U.B.

*Programming languages used*: FORTRAN IV

*High speed store required*: 12 608 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1679

*Keywords descriptive of problem and method of solution*: Atomic, Nuclear, Structure, Scattering, Recoupling Coefficient, Racah Coefficient, Wigner Coefficient, Fano Coefficient, Rotation Group, 3-*j* Symbol, 6-*j* Symbol, 9-*j* Symbol, 12-*j* Symbol, 15-*j* Symbol, 18-*j* Symbol, 21-*j* Symbol, Angular Momentum, Matrix Element, Angular Integral, Representation Of Three Dimensional Rotation.

*Nature of physical problem*

A general recoupling coefficient for an arbitrary number of integer or half integer angular momenta is calculated. The result is given as a floating point number.

*Method of solution*

The recoupling coefficient is first expressed as a sum over products of Racah coefficients multiplied by $(-1)$ factors and $(2j+1)^{1/2}$ factors. This summation is then evaluated.

*Restrictions on the complexity of the problem*

The program can be used to calculate a recoupling coefficient containing any number of angular momenta by modifying the dimensions of certain arrays.

*Typical running time*

The test run, consisting of four recoupling coefficients with between 3 and 7 angular momenta, takes 4 seconds to execute on the I.C.L. 1907 (this is approximately equivalent in speed to the IBM 7090).

*Unusual features of the program*

When the program has been used once to evaluate a given recoupling coefficient, it is possible to call the routine over and over again for the same coefficient with different angular momenta without re-expressing the recoupling coefficient in terms of Racah coefficients.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 265-276. NORTH-HOLLAND PUBLISHING COMPANY

# SINGLE-PARTICLE SUBSTITUTION SUMS IN THE SECOND-ORDER Z-EXPANSION THEORY OF ATOMIC ENERGIES*

M. N. LEWIS
*Harvard College Observatory, Cambridge, Massachusetts* 02138, *USA*

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): SPSS-ATOMIC Z-EXPANSION E2 PRIME

*Catalogue number*: AACC

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6400. *Installation*: Smithsonian Astrophysical Observatory, Cambridge, Massachusetts 02138, USA

*Operating system or monitor under which the program is executed*: SCOPE

*Programming languages used*: FORTRAN

*High speed store required*: 47,000 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer; Card Punch

*No. of cards in combined program and test deck*: 1911

*Keywords descriptive of problem and method of solution*: Atomic Theory, $Z$-Expansion, Second-order Perturbation Theory, Single Particle Substitution Sums, Hydrogenic Waves Functions, $n$-Expanded Wave Function, Slater $R^k$ Integrals.

*Nature of physical problem*

Program SPSS computes the single-particle substitution sums, $E_2'$, in the second-order term [1] in the $Z$-expansion theory of the energies of many-electron atoms.

The non-relativistic energy $E$ of atoms may be expanded by means of perturbation theory as the series in the nuclear charge $Z$, of the form

$$E = E_0Z^2 + E_1Z + E_2 + \dots, \quad \text{with} \quad E_2 = E_2' + E_2'' ,$$

where $E_2'$ is the single-particle substitution sum and $E_2''$ is the two-particle substitution sum.

*Method of solution*

$E_2'$ is calculated as one, or the sum of several, generalized sums $S_n'$ which may be given in the form of squares or product pairs of brackets containing one or several $R^k$ integrals over an energy denominator.

One wave function, $(nl)$, in each $R^k$ integral is a member of a complete set of hydrogen wave functions. The generalized sums $S_n'$ are found by straightforward summation over a limited range for $n$ up to $n = n_{\text{ext}} - 1$, by extrapolation from $n = n_{\text{ext}}$ to infinity, and integration over the continuum energy.

*Restrictions on complexity*

The restrictions on the principal quantum numbers $n_\alpha$ for the fixed wave functions depend on the precision desired, and the value used for $n_{\text{ext}}$. For $n_\alpha > 3$, double precision has been used with $n_{\text{ext}} = 160$. No results have been obtained for $n_\alpha > 12$.

*Typical running time*

Typical running times for $S_n'$ with one $R^k$ integral and 9-figure results are roughly: 1-2 seconds, single precision ($n_\alpha < 3$); 5-10 seconds, double precision ($n_\alpha > 3$).

*Unusual features of program*

Any combination of $R^k$ integrals (multiplied by coefficients), may be used, subject to the limits set by the dimension statements. The precision is controlled by an input parameter, and lack of convergence in integration or extrapolation is indicated by an asterisk following the numerical result.

*Reference*

[1] D. Layzer, Z. Horak, M. N. Lewis and D. Thompson, Ann. Phys. (N.Y.) 29 (1964) 101.

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* This work was supported by the National Science Foundati

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 277-280. NORTH-HOLLAND PUBLISHING COMPANY

# ISOMETRIC REPRESENTATION OF TWO-DIMENSIONAL MATRICES

A. CHOUDRY
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*Kingston, Rhode Island* 02881, *USA*

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): MATPLT

*Catalogue number*: ACQM

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/50, *Installation*: U.R.I., Kingston, R.I. 02881, USA

*Operating system or monitor under which the program is executed*: RAX

*Programming languages used*: FORTRAN IV, Level E

*High speed store required*: 13 224 words. *No. of bits in a word*: 8

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Benson-Lehner Graph Plotter

*No. of cards in combined program and test deck*: 107

*Keywords descriptive of problem and method of solution*: Isometric, 3-D Plot

*Nature of physical problem*

Quite frequently the numerical results of a theoretical calculation, as also the data from an experiment, are obtained in the form of a table or matrix, which describes a two-dimensional distribution of a physical quantity, e.g. charge distribution on a plate, neutron flux on the surface of a large detector, etc. In order to visually survey the entire data at a glance, the ideal presentation would be a three-dimensional model of the distribution in which the height, for example, corresponds to the value of the physical quantity. A similar visual effect can be obtained by a two-dimensional plot having a $45^{\circ}$ perspective and confirming to the optical constraint that visually hidden parts of the distribution are not drawn.

*Method of solution*

A main driver program computes or reads in the two-dimensional array to be plotted which is already specified to be in a common block. The main program now calls a FORTRAN subroutine MATPLT which retrieves the array from the common block and generates a deck of punched cards as output. The punched output contains instructions for an off-line plotter to plot the columns of the input matrix as histograms. Each successive column is plotted with 'shifted' origin. Furthermore before plotting a bin a check is made to see if the bin is obscured by the already plotted part of the distribution.

*Typical running time*

To generate plotter input for a typical 50 × 50 matrix it takes approximately one minute including compilation on an IBM 360/50 computer. The plotter instructions were generated for a Benson-Lehner digital plotter.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 281-290. NORTH-HOLLAND PUBLISHING COMPANY

# THE MADELUNG POTENTIAL AND ELECTRIC FIELD INTENSITY FOR A SODIUM CHLORIDE AND FOR A CAESIUM CHLORIDE LATTICE

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*The Queen's University of Belfast, BT7 1NN, Northern Ireland*

and

R. F. WOOD
*Solid State Division, Oak Ridge National Laboratory,*
*Oak Ridge, Tennessee 37830, USA*

Received 20 February 1970

## PROGRAM SUMMARY (NaCl LATTICE)

*Title of program*: NA CL MADELUNG FIELD

*Catalogue number*: ACMA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL 1907; 1900 series. *Installation*: Queen's University, Belfast, Northern Ireland

*Operating system or monitor under which the program is executed*: Queen's University of Belfast Operating System

*Programming languages used*: FORTRAN

*High speed store required*: 3584 words. *No. of bits in a word*: 24

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 267

*Keywords descriptive of problem and method of solution*: Solid State Physics, Electrostatic Potential, Madelung, Electrostatic Field, NaCl Lattice, Cubic Lattice, Point Charge, Evjen.

*Nature of physical problem*
This version of subroutine MDLG calculates the electrostatic potential and the components of the electrostatic field at an arbitrary point in space within an infinite array of positive and negative point charges arranged in the form of a NaCl-type lattice.

*Method of solution*
The direct summation method due to Evjen [1].

*Restrictions on the complexity of the problem*
The subroutine will not deal with a distorted lattice. Not more than one of the point charges may have a value different from that appropriate to the perfect lattice.

*Typical running time*
On the ICL 1907 machine, about 0.0024 $(2l+1)^3$ second for each call of the subroutine, where $l (\leq 8)$ is the number stored in L (see long write-up and listing for the definition).

*Unusual features of program*
Provision has been made to avoid failure or loss of accuracy through division by zero or a very small number if the point at which the results are required is too close to one of the point charges.

*Reference*

[1] H. M. Evjen, Phys. Rev. 39 (1932) 675.

## PROGRAM SUMMARY (CsCl LATTICE)

*Title of program*: CSCL MADELUNG FIELD

*Catalogue number*: ACMB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL 1907; 1900 series. *Installation*: Queen's University, Belfast, Northern Ireland

*Operating system or monitor under which the program is executed*: Queen's University of Belfast Operating System

*Programming languages used*: FORTRAN

*High speed store required*: 3712 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 299

*Keywords descriptive of problem and method of solution*: Solid State Physics, Electrostatic Potential, Madelung, Electrostatic Field, CsCl Lattice, Cubic Lattice, Point Charge, Evjen.

*Nature of physical problem*

This version of subroutine MDLG calculates the electrostatic potential and the components of the electrostatic field at an arbitrary point in space within an infinite array of positive and negative point charges arranged in the form of a CsCl-type lattice.

*Method of solution*

The direct summation method due to Evjen [1].

*Restrictions on the complexity of the program*

The subroutine will not deal with a distorted lattice. Not more than one of the point charges may have a value different from that appropriate to the perfect lattice.

*Typical running time*

On the ICL 1907 machine, about 0.0007 $(2l+1)^3$ second for each call of the subroutine, where $l$ ($\leqslant 10$) is the number stored in L (see long write-up and listing for the definition).

*Unusual features of program*

Provision has been made to avoid failure or loss of accuracy through division by zero or a very small number if the point at which the results are required is too close to one of the point charges.

*Reference*

[1] H.M.Evjen, Phys. Rev. 39 (1932) 675.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 293-305. NORTH-HOLLAND PUBLISHING COMPANY

# STLPLT - CALCOMP PLOT OF CRYSTALLOGRAPHIC PROJECTIONS OF LAUE PHOTOGRAPHS *

Marisa CANUT-AMOROS
*Materials Science, Southern Illinois University, Carbondale, Illinois, USA*

Received 20 May 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): STLPLT

*Catalogue number*: AASA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 7044; IBM 360/50 (after minor changes). *Installation*: Southern Illinois University.

*Operating system or monitor under which the program is executed*: IBSYS

*Programming languages used*: FORTRAN IV

*High speed store required*: 40 000 words. *No. of bits in word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: Besides the system read and write tapes, a tape for the CalComp and (optional) an input data tape.

*What other peripherals are used?* Card reader; Printer; CalComp Plotter System 470/556

*No. of cards in combined program and test deck*: 909

*Keywords descriptive of problem and method of solution*: Crystallography, Metallography, Laue Method, Stereographic and Gnomonic Projections.

*Nature of physical problem*

The program is designed to evaluate and plot the stereographic, stereognomonic and gnomonic projections from Laue photographs obtained with cylindrical, flat transmission or back reflection techniques.

*Method of solution*

From the $x$, $y$ coordinates of the Laue spots measured on the film, the $\rho$, $\phi$ and the $X$, $Y$ coordinates of the poles are calculated for the stereographic, stereognomonic or gnomonic projections. Cylindrical, flat transmission, or back-reflection Laue techniques can be used. The selected projection is plotted in a circle of 100 mm radius for any desired radius of the reference sphere. The blind zones of the experimental record determined by the film size and the backstop are also plotted on the projection.

*Typical running time*

On the IBM 7044 at Southern Illinois University the loading and assembly of the program requires 1.50 minutes. The execution time is dependent on the number of Laue spots. The execution time for the test run with the three plots was 2 minutes, 5 seconds. The plotting time on the CalComp plotting system 470/565 at the Materials Science Laboratory for two maps of the test run was 4 minutes.

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* Supported in part by the Solid State Sciences Division of the Air Force Office of Scientific Research, Grant AF-AFOSR-67-0832B.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 306-324. NORTH-HOLLAND PUBLISHING COMPANY

# A COMPUTER PROGRAM FOR THE CALCULATION OF ELECTRON SCATTERING AND PHOTOIONIZATION CROSS SECTIONS OF ATOMIC SYSTEMS WITH CONFIGURATION $(np)^q$ *

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*Behlen Laboratory of Physics and Department of Computer Science*
*University of Nebraska, Lincoln, Nebraska, USA*

P. G. BURKE
*Queen's University, Belfast, Northern Ireland*

and

R. J. W. HENRY
*Louisiana State University, Baton Rouge, Louisiana, USA*

Received 10 April 1970

## PROGRAM SUMMARY

*Title of program*: ATOMNP

*Catalogue number*: AAIA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/65. *Installation*: University of Nebraska, Computing Center.

*Operating system or monitor under which the program is executed*: OS 360

*Programming languages used*? FORTRAN IV

*High speed store required*: 31 000 words. *No. of bits in word*: 64

*Is the program overlaid*? Yes

*No. of magnetic tapes required*: 2

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 4320

*Keywords descriptive of problem and method of solution*: Atomic, Close-Coupling, Scattering, Photoionization, Cross Section, Electron, Atom, Coupled Differential Equation, Numerov, Fractional Parentage Coefficient, Clebsch–Gordon Coefficient, Racah Coefficient, Transition, Continuum Hartree–Fock, Wave Function, Schrödinger Fquation.

*Nature of Physical problem*

This program allows one to study the scattering of an electron by an atom or ion with configuration $(np)^q$, where $n = 2$ or 3, and $0 \leq q \leq 6$, under the assumption that all the ground state terms are "closely coupled", but no excited terms contribute [1-3].

*Method of solution*

It is similar to the Hartree–Fock method for bound states in that the total wave-function of the system is diagonal in total orbital angular momentum $L$, total spin $S$, and parity $\pi$, and is represented by a sum of Slater determinants. The wave functions for the core electrons are represented by analytic SCF functions of the form [4]

$$P_i = \sum_{\alpha} C(i,\alpha) r^{I(i,\alpha)} \exp[-\xi(i,\alpha) r] ,$$

where $i$ = 1s, 2s, 2p, .... The variation of the radial

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* Work supported by National Science Foundation and the Science Research Council.

functions $F_i$ for the continuum electron results in a set of $N$ coupled integro-differential equations of the following form.

$$\frac{d^2F_i(r)}{dr^2} = \sum_{j=1}^{N} A_{ij}(r)F_j(r) + \frac{2}{E - E_{N+1}} V_i(r) \int \sum_{j=1}^{N} V_j(r')F_j(r')dr' \div \sum_{K=1}^{NE} a_K y_{\lambda_K}(P_K F_K; r)P_K(r) + \sum_{j} \mu_i^j \delta_{l_i l_j} P_{l_j} : \qquad (1)$$

Given $L$, $S$, $\pi$ the code sets up the system of coupled equations for the atom or ion being considered and solves them by the numerical method described in ref. [1] (hereafter abbreviated as SHB).

The $R$-matrix, and hence the $S$-matrix, for the collision is obtained from the asymptotic form of these equations and multichannel photo-ionization cross sections are computed, if required, as formulated by Henry and Lipsky [5].

*Typical running time*

The time required depends on $N$, the number of equations, and on NE, the number of exchange terms. For electron-carbon scattering with $N = 2$, NE = 7 ($L = 0$, $S = \frac{1}{2}$, $\pi$ = even), the time required on the IBM 360/65 is 0.96 minutes. For the case $L = 2$, $S = \frac{1}{2}$, $\pi$ = even, we have $N = 5$, NE = 19 and the time required is 5.05 minutes.

*Unusual features of the program*

To obtain sufficient accuracy for numerical stability double precision is required on the IBM 360 series. This has not been necessary when using machines with 36 bit words.

*References*

[1] K. Smith, R. J. W. Henry and P. G. Burke, Phys. Rev. 147 (1966) 21.

[2] M. J. Seaton, in: Lectures in theoretical physics, Vol. IV, ed. Wesley E. Brittin (Interscience, New York, 1962).

[3] K. Smith, M. J. Conneely and L. A. Morgan, Phys. Rev. 177 (1969) 196;
R. J. W. Henry, P. G. Burke and A -L. Sinfailam, Phys. Rev. 178 (1969) 218.

[4] C. C. J. Roothaan, Rev. Mod. Phys. 32 (1960) 179;
C. C J. Roothaan, L. M Sachs and A. W. Weiss, Rev. Mod. Phys. 32 (1960) 186;
E. Clementi, Tables of atomic functions (IBM Research Laboratory, San Jose, 1963).

[5] R. J. W. Henry and L. Lipsky, Phys. Rev. 153 (1967) 51.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 325-336. NORTH-HOLLAND PUBLISHING COMPANY

# HYDROGENIC $R^k$ INTEGRALS *

M. N. LEWIS

*Harvard College Observatory, Cambridge, Massachusetts* 02138, *USA*

Received 22 December 1969

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): RKDP-RK INTEGRALS (DOUBLE PREC.)

*Catalogue number*: AACB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6400. *Installation*: Smithsonian Astrophysical Observatory, Cambridge, Massachusetts 02138, USA

*Operating system or monitor under which the program is executed*: SCOPE

*Programming languages used*: FORTRAN

*High speed store required*: 53000 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1373

*Keywords descriptive of problem and method of solution*: Slater $R^k$ Integral, Hydrogenic, Variable $Z$, Continuum $R^k$ Integral, Expanded Wave Function, Hydrogenic $Y^k$.

*Nature of physical problem*

Program RKDP presents a set of subroutines for double precision calculations of the sensitive parts of computations of Slater $R^k$ integrals with screened $Z$ hydrogenic wave functions. Three of the wave functions in the integral must be discrete and the fourth one can be discrete, continuum, or expanded. This set of subroutines may be used in program SPSS [1] for double precision calculations.

*Method of solution*

Analytic expressions for the wave functions, the $Y^k$ function and the integrals are used. The closed form of the expression for the $R^k$ integral is derived in ref. [2]. The derivation of the expanded form is given here. Values of the integrals computed with the closed and series expressions are compared.

*Restrictions on the complexity of the problem*

Space restrictions limit $n_1 + n_2 + n_3 + l_4 < 25$. Loss of significant figures limits the expansion of integrals approximately to those with $n_2 \leq 12$.

*Typical running time*

The typical running time for an individual $R^k$ integral is several milliseconds. The time required depends upon the quantum numbers.

*Unusual features of the program*

$R^k$ integrals of hydrogenic wave functions with screened $Z$'s can be checked by comparing results from two expressions.

*References*

[1] M. N. Lewis, Computer Phys. Commun. 1 (1970) 265.
[2] D. Layzer, Z. Horak, M. N. Lewis and D. Thompson, Ann. Phys. (N.Y.) 29 (1964) 101.

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* This work was supported by the National Science Foundation.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 337-342. NORTH-HOLLAND PUBLISHING COMPANY

# ANGULAR MOMENTUM COUPLING COEFFICIENTS

Taro TAMURA
*Center for Nuclear Studies, University of Texas, Austin, Texas 78712, USA*

Received 31 March 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): GEOMETRICAL COEFFICIENT

*Catalogue number*: ABMA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: Univ. of Texas Computation Center

*Operating system or monitor under which the program is executed*: CDC Scope

*Programming languages used*: FORTRAN IV

*High speed store required*: 5358 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card reader and lineprinter for driver

*No. of cards in combined program and test deck*: 342

*Keywords descriptive of problem and method of solution*: Nuclear, Atomic, Nuclear Spectra, Nuclear Structure, Atomic Spectra, Atomic Structure, Angular Momentum, Matrix Element, Transformation Matrices, Recoupling Coefficient, Racah Coefficient, Wigner Coefficient, Fano Coefficient, 3-*j*, 6-*j*, 9-*j*, Symbols, Clebsch—Gordan Coefficient.

*Nature of the physical problem*

Calculates the geometrical coefficients, like the Clebsch—Gordan coefficient, Racah coefficient, 9-*j* symbol and so forth, occurring in the quantum theory of angular momentum. The present program will thus be of universal use in almost any branch of physics that uses quantum mechanics.

*Method of solution*

Logarithms of factorials are calculated and are stored, once and for all in the beginning of the main routine. Symmetry properties of the coefficients are used to optimize the speed of the calculation.

*Restrictions on the complexity of the problem*

Restrictions come solely from the size of the core assigned to store the logarithms of factorials. Since the number of cores needed for that purpose is rather small in general, it does not mean in practice any real restriction. Also essentially there is no danger of over and underflow difficulties even when very large angular momenta are treated.

*Typical running time*

The running time is the longer the larger is the smallest argument that appears in a given coefficient. For the Clebsch—Gordan and Racah coefficients that are encountered in the usual calculations, with the values of arguments ranging from zero to twenty, say, the average time to calculate one of such coefficients is about one to two tenths of a millisecond on a CDC 6600.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 343-348. NORTH-HOLLAND PUBLISHING COMPANY

# SYMMETRIC NÉEL WALLS IN THIN MAGNETIC FILMS

A. HUBERT

*Max-Planck-Institut für Metallforschung, Institut für Physik, Stuttgart, Germany*

Received 31 March 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): SYMMETRIC NÉEL WALLS

*Catalog number*: ACKB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600; Telefunken TR4. *Installation*: Regionales Rechenzentrum Stuttgart, Germany; Rechenzentrum der Universität Stuttgart, Germany

*Operating system or monitor under which the program is executed*: CDC 6600 Scope 3.2

*Programming languages used*: ALGOL 60

*High speed store required*: 16500 words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card reader, Line printer

*No. of cards in combined program and test deck*: 424

*Keywords descriptive of problem and method of solution*: Micromagnetism, Magnetic Thin Films, Lorentz Microscopy, Domain Walls, Néel Walls, Ritz's Method.

*Nature of physical problem*

In very thin magnetic films a domain wall type may occur which is characterized by the rotation of the magnetization direction in the plane of the film. The structure of these so-called Néel-walls depends essentially on four external parameters: the film thickness, the total wall rotation angle (connected with the value of the applied field) and two anisotropy constants characterizing the material. Both uniaxial and multiaxial anisotropy may thus be represented. The calculation of these walls yields the wall energies, the detailed wall structure, the characteristic wall widths in the core and the tail regions of the walls, and Aharoni's self-consistency parameter [1].

*Method of solution*

The walls are calculated by Ritz's method with a one-dimensional ansatz similar to that used in [2]. This method has proved to give energies less than 1% higher than the exact result [3,4]. The starting values of the variational procedure may be automatically computed by the program.

*Restrictions on the complexity of the problem*

The present program calculates only isolated walls in an infinite film. The investigation of interacting walls is being prepared. So far the results should only be applied to cases where the walls are separated further than the external wall width calculated in the program. No net magnetic charge is allowed on the walls. The magnetic anisotropy must be a symmetric function of the magnetization component perpendicular to the wall and must be describable to sufficient accuracy by second and fourth order terms in this component.

*Typical running time*

One wall needs between 20 sec and 60 sec on the TR4 and approximately one third of this time on the CDC 6600. The higher running times are needed if the second anisotropy constant does not vanish.

*References*

[1] A. Aharoni, J. Appl. Phys. 39 (1968) 861.
[2] E. Feldtkeller, Z. Angew. Phys. 15 (1963) 206.
[3] R. Kirchner and W. Döring, J. Appl. Phys. 39 (1968) 855.
[4] A. Holz and A. Hubert, Z. Angew. Phys. 26 (1969) 145.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 349-358. NORTH-HOLLAND PUBLISHING COMPANY

# I. PROGRAM FOR CALCULATING DEGENERATE RAMAN BANDS OF SYMMETRIC TOPS WITH AN ADAPTATION FOR INFRARED BANDS *

F. N. MASRI
*Physics Department, University of Tennessee, Knoxville, Tennessee, USA*

and

I. R. WILLIAMS
*Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA*

Received 25 February 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): VIBROT I

*Catalogue number*: AAGC

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/65. *Installation*: University of Tennesse, Knoxville, Tennessee, USA

*Operating system or monitor under which the program is executed*: CO-OP

*Programming languages used*: ALGOL

*High speed store required*: 6 900 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* 2501 Card Reader; 1403 IBM-Printer

*No. of cards in combined program and test deck*: 300

*Keywords descriptive of problem and method of solution*: Molecule, Raman, Scattering, Spectra, Symmetric Tops, Coriolis Coupling.

*Nature of physical problem*

The program VIBROT I calculates the degenerate vibration–rotation bands of symmetric top molecules in the gas-phase infrared or Raman spectrum. Where only the band envelope is resolved, the program may be used to estimate band constants, such as the Coriolis constant $\zeta$, by a trial method using comparisons of observed and calculated spectra. Where the rotational fine structure is partially resolved, such a program may be necessary to assign features in the band and to determine accurate values of the band constants.

*Form of the program*

The modular structure of the program enables the use of alternative convolution procedures and the extension of the energy level calculation to higher order terms by a small modification of the appropriate procedures. The program has also been translated into FORTRAN IV.

*Restriction on the complexity of the program*

Bands involved in resonances, where a perturbation calculation is required, may not be calculated with the program.

*Typical running time*

The test case requires 1 minute 30 seconds to compile and run on the IBM 360/65 computer at the University of Tennessee.

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* Research sponsored in part by the U.S. Atomic Energy Commission under contract with the Union Carbide Corporation.
1969 Oak Ridge Associated Universities Research Participant from Knoxville College, Knoxville, Tennessee.

## ADAPTATION SUMMARY

*Title of adaptation* (32 characters maximum): ADAPT VIBROT I FOR INFRARED

*Adaptation number*: 0001

*Reference to original program*: *Catalogue number*: AAGC; *Title*: VIBROT I; *Ref. in CPC*: 1 (1970)

*Authors of original program*: F. N. Masri and I. R. Williams

*No. of cards required to effect adaptation* (including directive cards): 33

*Additional keywords, if applicable, descriptive of problem and method of solution*: Infrared, Absorption.

*Nature of the adaptation*

A direct interchange of a section of the inner block of the program allows the calculation of infrared bands in place of Raman bands.

*Typical running time*

The test case requires 30 seconds to compile and run on the IBM 360/65 Computer at the University of Tennessee.

COMPUTER PHYSICS COMMUNICATIONS 1 (1969) 359-377. NORTH-HOLLAND PUBLISHING COMPANY

# A GENERAL PROGRAM FOR CALCULATING ANGULAR MOMENTUM INTEGRALS IN ATOMIC STRUCTURE

A. HIBBERT
*Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Northern Ireland*

Received 7 January 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): WEIGHTS

*Catalogue number*: ACQL

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL 1907. *Installation*: Queen's University, Belfast, N.I.

*Operating system or monitor under which the program is executed*: QUBE

*Programming languages used*: FORTRAN IV

*High speed store required*: 30 K words. *No. of bits in a word*: 24

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer; Card Punch (Optional)

*No. of cards in combined program and test deck*: 2043

*CPC Library subprograms used*

| *Catalogue numbers* | *Titles* | *Refs. in CPC* |
|---|---|---|
| ACQB | P SHELL C.F.P. | 1 (1969) 15 |
| ACQC | D SHELL C.F.P. | 1 (1969) 16 |
| AAGD | NJSYM | 1 (1970) 241 |

*Keywords descriptive of problem and method of solution*: Atomic, Configuration Interaction, Racah, Coefficients Of Fractional Parentage, Recoupling Coefficients, Slater Integrals, Complex Atoms, Wave Function, Bound States, *LS* Coupling.

*Nature of physical problem*

In configuration interaction calculations, one wishes to evaluate the matrix of the Hamiltonian operator with respect to a basis set of configuration wave functions. The more difficult part of this procedure is the determination of the two-electron interaction matrix elements. These matrix elements may be written as a weighted sum of radial Slater integrals. The program calculates the coefficients of these integrals.

*Method of solution*

The coefficients of the Slater integrals are obtained from integration over all spin and angular co-ordinates and $(N-2)$ radial co-ordinates, for an $N$-electron atom. The scheme for calculating the coefficients is described by Fano [1], using the techniques of Racah [2]. In this scheme, the coefficients may be expressed as sums over fractional parentage coefficients (Allison [3]), recoupling coefficients (Burke [4]), and reduced matrix elements (Fano and Racah [5]).

The configurations are defined by the number of electrons in each occupied shell, and the $(nl)$ quantum numbers and angular momentum couplings for each occupied shell.

*Restrictions on the complexity of the problem*

Any number of electrons in s-, p-, or d-shells are allowed ($\leq 2(2l+1)$), but no more than two electrons in any shell of higher orbital angular momentum. This restriction may be relaxed by inclusion of further fractional parentage coefficient packages.

*References*

[1] U. Fano, Phys. Rev. 140 (1965) A67.
[2] G. Racah, Phys. Rev. 63 (1943) 367.
[3] D. C. S. Allison, Computer Phys. Commun. 1 (1969) 15.
[4] P. G. Burke, Computer Phys. Commun. 1 (1970) 241.
[5] U. Fano and G. Racah, Irreducible tensorial sets (Academic Press, New York, 1959) p. 81.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 380-390. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTATION OF CHARGE TRANSFER PROBABILITY BETWEEN PROTONS AND EXCITED HYDROGEN ATOMS

V. MALAVIYA *
*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, Northern Ireland*

Received 20 August 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): $H^+$+H(2) CHARGE TRANSFER

*Catalogue number*: ACQQ

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL 1907. *Installation*: Queen's University of Belfast

*Operating system or monitor under which the program is executed*: QUBE

*Programming languages used*: FORTRAN

*High speed store required*: 24 512 words. *No. of bits in a word*: 24

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1054

*Keywords descriptive of problem and method of solution*: Atomic, Schrödinger Equation, Impact Parameter, One-electron Wavefunction, Charge Transfer, Momentum Transfer, Overlap and Interaction Matrices, Matrix Inversion, Perturbed Energies, LCAO Approximation, Molecular States, Cross Section, First-order Linear Partial Differential Equations.

*Nature of physical problem*

The program simultaneously computes momentum transfer matrix elements and excitation and charge transfer probabilities for collisions between protons and hydrogen atoms in the second quantum levels in any of the three molecular states associated with the second quantum level of the hydrogen atom. The alternative procedure using direct numerical integration is also discussed and developed.

*Method of solution*

The exchange matrix elements are evaluated by solving a set of coupled differential equations suggested by Cheshire [1]. The differential equations relating the transition amplitudes are combined with the differential equations relating the matrix elements, and are solved by the Adams-Moulton method.

*Typical running time*

The time required to compute the probability for a given energy and impact parameter depends upon the energy, and increases rapidly as the energy is decreased. For example, for an energy of 10 KeV, the time is 300 sec for any impact parameter but for an energy of 500 eV, it is 1800 sec.

*Reference*

[1] I. M. Cheshire, Proc. Phys. Soc. (London) 92 (1967) 862.

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* On leave of absence from the Department of Applied Physics, University of Allahabad, Allahabad, India.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 391-414. NORTH-HOLLAND PUBLISHING COMPANY

# POLYMOL: A GENERAL PROGRAM FOR THE CALCULATION OF GROUND-STATE WAVE FUNCTIONS OF POLYMERS

Jean-Marie ANDRE
*IBM Research Laboratory, Monterey and Cottle Roads, San José, California* 95114, *USA*
*and Laboratoire de Chimie Quantique*, 3030-*Heverlee, Belgium*

Received 7 May 1970

## PROGRAM SUMMARY

*Title of program*: POLYMOL

*Catalogue number*: ABYA

*Computer for which the program is designed and others upon which is is operable*

*Computer*: IBM 360/91. *Installation*: IBM Research laboratory, San José, USA

*Operating system or monitor under which the program is executed*: OS360

*Programming languages used*: FORTRAN IV

*High speed store required*: 55 112 words. *No. of bits in word*: 32

*Is the program overlaid*? Yes

*No. of magnetic tapes required*: 3

*What other peripherals are used*? Disk unit 2314; card reader; line printer

*No. of cards in combined program and test deck*: 6789

*Keywords descriptive of problem and method of solution*: Quantum Chemistry, Polymer, Crystal, Molecule, Closed Shells, Band Structure, Ground State, Wave Function, Singlet, Gaussian Orbitals, Hartree-Fock, Bloch Orbitals, Self-Consistent Field, IBMOL, One-electron Integral, Two-electron Integral.

*Nature of physical problem*

POLYMOL is an SCF LCGO program, designed for computing the all-electrons band structure of periodic polymers. The program handles only closed shells.

*Method of solution*

Self-consistent field method within the framework of LCAO approximation and Bloch theorem.

*Restrictions on the complexity of the problem*

Only singlet wave functions can be handled by the POLYMOL program. When restricted to 30 atomic orbitals per unit cell, the maximum length of the overlaid program is $(330F0)_{16} = (209136)_{10}$ bytes. An extended version, allowing up to 80 atomic functions per unit cell is running in a 512K core memory.

*Typical running time*

The time for the test case (idealized polyethylene in the nearest neighbor approximation) is 27 minutes for a basis of 4 s-type and 2 p-type gaussians for the carbon atom (4s - 2p basis) and 1 gaussian of s-type for the hydrogen atom. Corresponding running time for a 7s - 3p basis for the carbon and 3s for the hydrogen is 177 minutes on an IBM 360/91.

*Unusual features of the program*

Some of the routines are written in IBM 360 Assembler language.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 415-419. NORTH-HOLLAND PUBLISHING COMPANY

# AN ALGORITHM GENERATING PERMUTATIONS WITH IDENTICAL OBJECTS

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*Centre de Physique Théorique, C.N.R.S., 31, Chemin J.Aiguier, 13 - Marseille (9e), France*

Received 29 June 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): PERMID

*Catalogue number*: ACQP

*Computer for which the program is designed and others upon which it is operable*

*Computer*: UNIVAC 1108. *Installation*: Faculté des Sciences, Orsay, France

*Operating system or monitor under which the program is executed*: EXEC II

*Programming languages used*: FORTRAN

*High speed store required*: 726 words. *No. of bits in a word*: 36

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 222

*Keywords descriptive of problem and method of solution*: Combinatorial Analysis, Permutations.

*Nature of the physical problem*

For a given set of $N$ objects where $\lambda_1, \lambda_2, \ldots, \lambda_p$ ones are identical, we give an algorithm which generates all the distinct permutations of the $N$ objects, without the necessity to store the permuted elements in order to compute the next ones. As an application of the algorithm we have written a FORTRAN subroutine generating these permutations.

*Method of solution*

In the case of distinct objects there exists the methods of group theory based upon cyclic permutations [1, 2]. When objects may be idential the previous methods no longer apply, and in this case we have defined an algorithm where the permutations are reduced to commutations of elements according to a set of three operatorial rules. The method is similar in some respects to the treatment of non commutative algebras [3].

*Restriction on the complexity of the problem*

The program is applicable to permute integer numbers, but this restriction is easily removed by making a one to one correspondance between the integers and a finite set of objects.

*Typical running time*

The running time depends on the number of objects and their repartition in identical groups. As an example: for 2520 permutations 0.326 second, for 332040 permutations 42.65 seconds.

*References*

[1] D. E. Rutherford, Substitutional analysis (The Edinburgh University Press, Edinburgh, 1948).
[2] D.E Knuth, The art of computer programming, Vol. 1, Fundamental algorithms (Addison-Wesley, Reading, 1968).
[3] C. Bourrely and F. Di Guglielmo, Rev. Française Inform. Rech. Oper. R-1 (1970) 81.

COMPUTER PHYSICS COMMUNICATION 1 (1970)420-424. NORTH-HOLLAND PUBLISHING COMPANY

# CONVERSION OF BINARY MAGNETIC TAPES

J. GOLDBERG
*Department of Physics, Technion - Israel Institute of Technology, Haifa, Israel*

Received 21 May 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): CONV

*Catalogue number*: ABCA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360. *Installation*: Technion, Haifa, Israel

*Operating system or monitor under which the program is executed*: OS

*Programming languages used*: FORTRAN IV and one ASM subroutine

*High speed store required*: 15K words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: 2 (1 seven tracks)

*What other peripherals are used*? Card Reader; Printer

*No. of cards in combined program and test deck*: 276

*Keywords descriptive of problem and method of solution*: Translation, Binary Tapes.

*Nature of physical problem*

Use of experimental results stored on tapes from other computers.

*Method of solution*

Automatic recognition of word structure, and word to word structure exchange.

*Restrictions on the complexity of the problem*

BCD words are incorrectly translated.

*Typical running time*

200 records of 500 words each per minute on IBM 360/50.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 425-436. NORTH-HOLLAND PUBLISHING COMPANY

# A MONTE CARLO GENERATION METHOD WITH IMPORTANCE SAMPLING FOR HIGH ENERGY COLLISIONS OF HADRONS

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*CERN, European Organisation for Nuclear Research, Geneva, Switzerland*

and

W. WOJCIK *
*CEN, Centre d'Etudes Nucléaires, Saclay, France*

Received 18 July 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): GENIS

*Catalogue number*: AAUA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600; all types with FORTRAN IV compiler. *Installation*: CERN, Geneva, Switzerland

*Operating system or monitor under which the program is executed*: CERN version of CDC SCOPE 2.0

*Programming languages used*: FORTRAN IV

*High speed store required*: 877 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripharals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 400

*Keywords descriptive of problem and method of solution*: Nuclear, High Energy, Hadron, Phase Space, Collision, Elementary Particle, Monte Carlo Integration, Importance Sampling, Restricted, Transverse Momenta.

*Nature of physical problem*

In the theoretical analysis of hadron collisions at high energies the numerical evaluation of integrals over complete phase space is wasteful of computer time because experiment shows that only a small region of the integration domain is relevant for most physical purposes. This region is characterised by small values of the transverse momenta of the particles produced in the collision.

*Method of solution*

We use a Monte Carlo integration method with importance sampling, taking as integration variables the momenta of the outgoing particles in the centre-of-mass system and distinguishing between their longitudinal and transverse components. The former increase with energy, the latter grow only at low energies and remain essentially constant at high energies [1].

*Restrictions on the complexity of the problem*

The program is designed for a number $n$ of outgoing particles of up to 18. This limit can be increased easily by the user if required.

*Typical running time*

The numbers in table 1 apply for the CDC 6600 computer at CERN. The first column gives the number of outgoing particles, the second the approximate computing time per generated point for points fulfilling the kinematic constraint (eq. (14) of long write-up). Except at low energy, practically all generated points satisfy the constraint. The rest of the table shows the percentage of generated points which violate it for two values of the energy, the latter being expressed in terms of the laboratory momentum $p_{\mathrm{LAB}}$ of the incident beam particle.

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* On leave from the Institute of Experimental Physics, University of Warsaw, Warsaw, Poland.

Table 1

| $n$ | Time/point in msec | $p_{LAB}$ in GeV/$c$ | perc. | $p_{LAB}$ in GEV/$c$ | perc. |
|---|---|---|---|---|---|
| 3 | 2 | 0.3 | 25% | 3.0 | 1% |
| 6 | 5 | 1.0 | 15% | 8.0 | 1% |
| 10 | 9 | 2.3 | 7% | 17.5 | 1% |
| 18 | 21 | 6.0 | 2% | 8.0 | 1% |

*Unusual features of the program*

GENIS is a subprogram to be used with any main program feeding it with the information on the incoming laboratory momentum and total energy in the centre of mass as well as the masses of incoming and outgoing particles. It is in particular suited to be used with FOWL [2].

*References*

[1] L. Van Hove, Nucl. Phys. B9 (1969) 331.
[2] F. James, FOWL, CERN Program Library (1970) W505.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 437-439. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM TO CALCULATE THE RADIAL PARTS OF INTERACTION MATRIX ELEMENTS BETWEEN TWO HYDROGENIC WAVE FUNCTIONS AS POWER SERIES

M. J. JAMIESON *

*Harvard College Observatory, Cambridge, Massachusetts, USA*

Received 17 August 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): HYDROGENIC INTERACTION INTEGRAL

*Catalogue number*: ABWA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6400. *Installation*: Smithsonian Astrophysical Observatory, Cambridge, Massachusetts

*Operating system or monitor under which the program is executed*: SCOPE

*Programming languages used*: FORTRAN

*High speed store required*: 9280 words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 281

*Keywords descriptive of problem and method of solution*: Atomic, Hydrogenic Wave Function, Radial Integral, Interaction, Matrix Element, Power Series.

*Nature of physical problem*

The study of the collisional excitation of atoms by charged projectiles involves interaction matrix elements of the form

$$V_{a,a'}(\boldsymbol{R}) = \int \phi_a^*(\boldsymbol{r}) \frac{1}{|\boldsymbol{r}-\boldsymbol{R}|} \phi_{a'}(\boldsymbol{r}) \mathrm{d}\boldsymbol{r} , \qquad (1)$$

where $\phi_a(\boldsymbol{r})$ is an orbital describing an atomic electron with position vector $\boldsymbol{r}$ relative to the nucleus, and $\boldsymbol{R}$ is the position vector of the charged projectile [1]. If $\phi_a(\boldsymbol{r})$ is expanded in hydrogenic wave functions the matrix element is reduced to a sum of expressions such as (1) with the $\phi$'s replaced by hydrogenic wave functions. An expansion of $1/|\boldsymbol{r}-\boldsymbol{R}|$ in spherical harmonics of $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{R}}$ [2] further reduces the integral to a sum of radial integrals involving hydrogenic wave functions, multiplied by functions of $\hat{\boldsymbol{R}}$.

*Method of solution*

The radial integrals are calculated analytically to yield power series in $R$.

*Restrictions on the complexity of the problem*

For large principal quantum numbers certain dimensions need to be increased.

*Typical running time*

Typically 0.2 seconds.

*References*

[1] M. J. Seaton, in: Atomic and molecular processes, ed. D. R. Bates (Academic Press, New York and London, 1962).
[2] A. Messiah, Quantum mechanics, Vol. 1 (North-Holland, Amsterdam, 1964) pp. 496, 497.

* Now at Department of Theoretical Chemistry, University of Cambridge, UK.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 440-444. NORTH-HOLLAND PUBLISHING COMPANY

# SPECTRAL INTENSITY, ANGULAR DISTRIBUTION AND POLARISATION OF SYNCHROTRON RADIATION FROM A MONOENERGETIC ELECTRON

James LANG
*Department of Natural Philosophy, The University, Glasgow W2, Scotland*

Received 17 September 1970

## PROGRAM SUMMARY

*Title of program*: SYNCHROTRON RADIATION

*Catalogue number*: ACQR

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL KDF9. *Installation*: (1) Glasgow University, Glasgow W2, Scotland
(2) Culham Laboratory, Abingdon, Berks., England

*Operating system or monitor under which the program is executed*: Egdon 3

*Programming languages used*: FORTRAN

*High speed store required*: 3000 words. *No. of bits in a word*: 48

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Line Printer, Card Reader

*No. of cards in combined program and test deck*: 321

*Keywords descriptive of problem and method of solution*: Atomic, Solid State, Synchrotron, Radiation, Polarisation, Angular Distribution, Intensity, Spectral Intensity, Absolute Intensity, Absolute Source, Radiometry, Relativistic Electron, Circular Orbit, Bessel Function, Series Solution, Integration.

*Nature of the physical problem*

The absolute power radiated by a relativistic electron travelling in a circular orbit in a synchrotron can be calculated theoretically. This program evaluates, for an electron of specified energy and orbit radius, the power radiated round the orbit

(a) as a function of wavelength (i.e. spectral distributions)

(b) as a function of the angle above or below the orbital plane at any particular wavelength. These angular distributions are given for the component polarised with $\boldsymbol{E}$-vector in a plane parallel to the orbital plane and for the component polarised with $\boldsymbol{E}$-vector in a plane perpendicular to the orbital plane.

*Method of solution*

The expressions used in the calculations are those given by Tomboulian and Hartman [1] and which were originally given by Schwinger [2] in a slightly different form. Olsen [3] and Westfold [4] have shown how the angular distribution formula also gives the polarisation. The equations contain Bessel functions of the second kind (McDonald functions) $K_n(S)$ of order $n$ which are calculated from series expansions. The spectral distributions involve the integration of functions of order 5/3 and the other distributions involve the squaring of functions of order 1/3 and 2/3.

*Restriction on the complexity of the problem*

The series method of solution of the Bessel functions means that the argument of Bessel function is prevented from exceeding six. For the spectral distributions the calculation is thus cut-off when the wavelength is 2.52 times down on the wavelength of peak power, the wavelengths higher than that of the peak power being unaffected. For the angular distributions at a fixed wavelength. The restriction introduces a cut-off as the angle above or below the orbital plane is increased. However, at this cut-off the power is down by at least two orders of magnitude on the power at the peak of the angular distribution.

*Typical running time*

The test case compiles in 22 seconds and takes 77 seconds to run on the Glasgow University KDF9.

*References*

[1] D.H.Tomboulian and P.L.Hartman, Phys.Rev. 102 (1956) 1423.
[2] J.Schwinger, Phys.Rev. 75 (1949) 1912.
[3] H.Olsen, Kgl.Norske Videnskab.Selskabs Skrifter (1952) nr. 5.
[4] K.C.Westfold, Astrophys.J. 130 (1959) 241.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 445-452. NORTH-HOLLAND PUBLISHING COMPANY

# ELECTRON SCATTERING BY CLOSED SHELL DIATOMIC MOLECULES

A. L. SINFAILAM
*Institute for Pure and Applied Physical Sciences ,*
*University of California, San Diego, La Jolla, California* 92037, *USA*

Received 7 August 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): ELECTRON-MOLECULE SCATTERING

*Catalogue number*: ACQO

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 3600. *Installation*: University of California, San Diego

*Operating system or monitor under which the program is executed*: PRESTO

*Programming languages used*: FORTRAN IV

*High speed store required*: 32 K Words. *No. of bits in a word*: 48

*Is the program overlaid*? Yes

*No. of magnetic tapes required*: None

*What other peripherals are used*? Scratch tape for overlay system

*No. of cards in combined program and test deck*: 6744

*Keywords descriptive of problem and method of solution*: Quantum Chemistry, Molecular Physics, Electron Scattering, Diatomic Molecule, Closed Shell Orbitals, Born-Oppenheimer Approximation, Single Centre Expansion, $K$-Matrix Eigenphases, Elastic Cross Section, Schrödinger Equation, Continuum Hartree Fock.

*Nature of physical problem*

A general computer code for studying the low energy electron scattering by closed shell diatomic molecule is presented. It is assumed that the molecule is constrained in its electronic state and does not vibrate or rotate during the collision. The $K$-matrix elements, the eigenphases and the elastic cross section are evaluated [1].

*Method of solution*

Our approach is based on a single centre expansion of the molecular and incident electron orbitals about the centre of mass of the molecule. The target molecule is represented by the Hartree-Fock molecular wave function. The adiabatic or Born-Oppenheimer approximation, which assumes that the molecular axis does not rotate during the collision, is used to describe the scattering process. The coupled integro-differential equations are solved using the method already discussed for electron atom collisions [2].

*Restrictions on the complexity of the program*

The program is designed to study the scattering by a closed shell diatomic molecule with sigma and pi orbitals. It can, however, be modified to treat higher orbitals and also to examine the scattering by a closed shell diatomic positive molecular ion. Moreover, the code can easily be adapted for the study of positron scattering by a linear molecule. The user must provide the molecular orbitals and the static potentials; these can be evaluated using, for example, the program of ref. [3].

*Typical running time*

Running time is proportional to $N^2$, where $N$ is the number of coupled equations. In the $^2\Pi_u\, e^- - N_2$ test case, $N = 20$ and the running time is 4 min. Compilation time is 3 min. These figures are for the CDC 3600 at the University of California at San Diego.

*References*

[1] P. G. Burke and A. L. Sinfailam, J. Phys. B3 (1970) 641.
[2] K. Smith, R. J. W. Henry and P. G. Burke, Phys. Rev. 147 (1966) 21.
[3] F. H. M. Faisal, A. L. Sinfailam and N. Turner, to be submitted to C.P.C.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 453-456. NORTH-HOLLAND PUBLISHING COMPANY

# ALLOWED VALUES OF COUPLED ANGULAR MOMENTUM AND i-SPIN FOR NUCLEONS IN A SINGLE SHELL IN $j$-$j$ COUPLING *

Lincoln B. HUBBARD
*Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA*
*and Knoxville College, Knoxville, Tennessee, USA*

Received 27 July 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): JNTJN

*Catalogue number*: ABKC

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM-360/75 and 91. *Installation*: Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

*Operating system or monitor under which the program is executed*: OS360

*Programming languages used*: FORTRAN-IV (H)

*High speed store required*: 16 500 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripharals are used?* Standard card-reader and printer

*No. of cards in combined program and test deck*: 204

*Keywords descriptive of problem and method of solution*: Nuclear, Angular Momentum, Wave Functions, $j$-$j$ Coupling, Shell Model.

*Nature of physical problem*

If there are a given number of nucleons in a single shell in $j$-$j$ coupling, there are only a restricted number of orthogonal eigenfunctions allowed by the exclusion principle. The program JNTJN calculates the number of allowed eigenfunctions in the representation of coupled i-spin and angular momentum; i.e., the number of eigenvectors for each pair of $T$ and $J$ values is calculated.

*Method of solution*

The program JNTJN enumerates the allowed values for the projections, $M_J$ and $M_T$, of the coupled angular momentum and i-spin. From these projections, the allowed eigenvalues of $J$ and $T$ are readily found. This is similar to the enumeration schemes in the literature [1,2].

*Restrictions on the complexity of the problem*

This program is applicable to the enumeration of the allowed values of total angular momentum and i-spin for any number of particles in any $j$-shell. Some modifications in printing and array dimensions would be necessary for calculations near the center of shells having $j \geq 13/2$.

*Typical running time*

The sample output required about one-tenth second on the IBM-360/91; compile time is about 1.5 seconds. The complete enumeration of the lower half of the $j$ = 3/2, 5/2, 7/2 and 9/2 shells required about 35 seconds of execution on the same machine.

*References*

[1] B. H. Flowers, Proc. Roy. Soc. A212 (1952) 248.
[2] A. de Shalit and I. Talmi, Nuclear shell theory (Academic Press, New York, 1963).

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* Research sponsored in part by the U.S. Atomic Energy Commission under contract with the Union Carbide Corporation.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 457-464. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM TO GENERATE NUMERICAL ORBITAL FUNCTIONS

W. D. ROBB
*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, BT7 1NN, Northern Ireland*

Received 17 September 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): NUMERICAL ORBITAL FUNCTIONS

*Catalogue number*: ACQS

*Computer for which the program is designed and others upon which it is operable*

| *Computer*: | *Installation*: |
|---|---|
| (1) CDC 6600 | (1) University of London, England. |
| (2) ICL 1907 | (2) Queen's University of Belfast, N. Ireland. |
| (3) ATLAS 1 | (3) Atlas Computer Laboratory, Chilton, Berks., England. |

*Operating system or monitor under which the program is executed*: SCOPE

*Programming languages used*: FORTRAN

*High speed store required*: 15360 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader, Line Printer

*No. of cards in combined program and test deck*: 844

*Keywords descriptive of problem and method of solution*: Atomic, Nuclear, Basis Functions, Continuum, Bound, Bessel Functions, Yukawa, Static, Square Well, De Vogelaere, $R$-matrix, Eigenfunction.

*Nature of physical problem*

The program BASFUN solves the radial Schrödinger equation for any specified central potential and angular momentum, either at a given energy, or subject to a given $R$-matrix [1] boundary condition. In both cases the solution can be made orthogonal to any number of specified functions.

The eigenfunctions which are obtained in numerical form are required:

(a) as continuum basis functions in an $R$-matrix calculation

(b) as Sturmian functions to be used in the calculation of atomic properties such as the van der Waals coefficient.

*Method of solution*

The differential equation is integrated using de Vogelaere's method [2], over intervals specified by the user. The eigenfunction and eigenvalue are found using Newton's iteration method, and orthogonality to the specified functions using the method of Lagrange undetermined multipliers and Simpson's rule.

*Restrictions on the complexity of the program*

The dimensions of the storage arrays give a restriction which may be changed by the user. The potential is restricted to a central spin-independent form

*Typical running time*

This depends on the number of functions to which the solution is orthogonalised, on the number of integration points used and on whether or not an eigensolution is required. The mill time for the test run on the CDC 6600 is 1.1 seconds.

*References*

[1] A. M. Lane and R. J. Thomas, Rev. Mod. Phys. 30 (1958) 257.
[2] W. A. Lester Jr., Univ. Wisconsin Theoret. Chem. Inst. Report WIS-ICI-285 (1968).

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 465-467. NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAM FOR FITTING TRANSITION ENERGIES INTO A LEVEL SCHEME ACCORDING TO THE COMBINATION PRINCIPLE *

I. R. WILLIAMS
*Knoxville College, Knoxville, Tennessee, USA*

Received 22 September 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): RITZ COMBINATION PRINCIPLE

*Catalogue number*: ABKD

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/91, SEL 840A. *Installation*: Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

*Operating system or monitor under which the program is executed*: S/360 OS(MVT)

*Programming languages used*: FORTRAN IV

*High speed store required*: 1 100 words. *No. of bits in word*: 32 (2 500 words and 24 bits for the SEL 840A)

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader, Line Printer

*No, of cards in combined program and test deck*: 113

*Keywords descriptive of problem and method of solution*: Nuclear, Atomic, Molecular, Spectra, Energy Level, Gamma Ray, Photon, Quantum, Ritz Combination Principle.

*Nature of physical problem*

In nuclear physics (but also in atomic and molecular physics) transition energies are often obtained from measurements of photon or internal electron conversion spectra. An attempt is then made to fit these energies into a level scheme (of which some levels may already be known) on the basis of the conservation of energy here termed the Ritz Combination Principle.

*Method of solution*

The essential input data are the measured photon energies and any level energies that are known. The program starts at a specified energy ($E$) and ascertains whether (a) an energy level (b) an energy level + a quantum (c) an energy level - a quantum or (d) a quantum + another quantum have that energy $E$ within experimental error (also specified input data). The value of $E$ is reduced a little and the program loops through the series of questions, again outputting the pertinent data if an answer is in the affirmative. This is repeated as long as desired; the output eventually having the semblance of an energy level diagram.

*Restrictions on the complexity of the problem*

This program takes no consideration of the fact that a transition between two levels may be forbidden because of an angular momentum and parity barrier. Also no intensity balance is accounted for in program RITZ so it is necessary to be on guard against accepting the program's assignment of a transition to a state in the decay scheme when this might be totally unreasonable from intensity considerations.

*Typical running time*

The total CPU time for the test case is 2.9 seconds. The running time goes up rapidly with the number of gamma level energies taken as input.

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* Research sponsored in part by the U.S. Atomic Energy Commission under contract with the Union Carbide Corporation.

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 468. NORTH-HOLLAND PUBLISHING COMPANY

# SYMMETRIC NEEL WALLS IN THIN MAGNETIC FILMS. AN ADAPTATION TO INCREASE THE RANGE OF CONVERGENCE

A. HUBERT
*Max-Planck-Institut für Metallforschung,*
*Institut für Physik, Stuttgart, Germany*

Received 8 September 1970

## ADAPTATION SUMMARY

*Title of adaptation* (32 characters minimum): INTERNAL IMPROVEMENTS

*Adaptation number*: 0001

*Reference to original program*: Catalogue number ACKB; Title: SYMMETRIC NEEL WALLS; Ref. in C.P.C. 1 (1970) 343.

*Author of original program*: A. Hubert

*No. of cards required to effect adaptation (including directive cards)*: 78

*Nature of the adaptation*

The adaptation consists of improvements to the internal organization to increase the range of convergence, particularly for high anisotropy ratios. Additional precautions have been introduced for the case of bad convergence. The output from the test run of this adaptation is essentially unaltered from that of the original program.

## ERRATUM NOTICES

*Title of manuscript*: Single-particle substitution sum in the second-order $Z$-expansion theory of atomic energies.

*Author*: M. N. Lewis

*Reference*: Computer Physics Communications 1 (1970) 265.

*Title of program*: SPSS-ATOMIC Z-EXPANSION E2 PRIME

*Catalogue number*: AACC

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*Title of manuscript*: Hydrogenic $R^k$ integrals

*Author*: M. N. Lewis

*Reference*: Computer Physics Communications 1 (1970) 325.

*Title of program*: RKDP-RK INTEGRALS (DOUBLE PREC.)

*Catalogue number*: AACB

COMPUTER PHYSICS COMMUNICATIONS 1 (1970) 470-472. NORTH-HOLLAND PUBLISHING COMPANY

# ERRATUM

M. J. Conneely, L. Lipsky, K. Smith, P. G. Burke and R. J. W. Henry, A computer program for the calculation of electron scattering and photoionization cross sections of systems with configuration $(np)^q$, Computer Physics Communications 1 (1970) 306.

The output from the test run was omitted by mistake and is reproduced below.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 11-16. NORTH-HOLLAND PUBLISHING COMPANY

# SYMMETRY AND BAND STRUCTURE
## I. SELECTION OF RECIPROCAL LATTICE VECTORS *

V. HOFFSTEIN ** and O. MOLLER ***
*Department of Physics, Polytechnic Institute of Brooklyn, Brooklyn, New York* 11201, *USA*

Received 30 June 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): SYMMETRY AND BAND STRUCTURE 1

*Catalogue number*: ACMD

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/50. *Installation*: Polytechnic Institute of Brooklyn

*Operating system or monitor under which the program is executed*: OS 360/50, WATFOR compiler

*Programming languages used*: FORTRAN IV

*High speed store requiree*: 61167 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 397

*Keywords descriptive of problem and method of solution*: Solid State, Band Structure, Symmetry, Symmetrized Plane Waves, Pseudopotential, Group Theory.

*Nature of the physical problem*
The first section of a program to perform the symmetry part of band structure calculations. This part selects a symmetry adapted set of reciprocal lattice vectors.

*Method of solution*
Expansion of the wave function in terms of symmetrized plane waves [1].

*Restrictions on the complexity of the problem*
Limited to cubic lattices.

*Typical running time*
3-7 minutes depending on the energy.

*Reference*

[1] A. W. Luehrmann, Advan. Phys. 17 (1968) 65, 1; Ph.D. thesis, University of Chicago (1967).

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* Work supported by the U.S. Air Force, Office of Scientific Research grant number: AFOSR-1709-69.
** Present address: Laboratoire de Spectrométrie Physique, CEDEX 53, 38-Grenoble-Gare, France.
*** Since the acceptance of this paper for publication Dr. O. Moller was tragically killed in an automobile accident.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 17-25. NORTH-HOLLAND PUBLISHING COMPANY

# SYMMETRY AND BAND STRUCTURE
## II. STORAGE AND RETRIEVAL OF GROUP THEORETICAL INFORMATION *

V. HOFFSTEIN ** and O. MOLLER ***
*Physics Department, Polytechnic Institute of Brooklyn, Brooklyn, New York* 11201, *USA*

Received 20 July 1970

*Title of program* (32 characters maximum): SYMMETRY AND BAND STRUCTURE 2

*Catalogue number*: ACME

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/50. *Installation*: Polytechnic Institute of Brooklyn

*Operating system or monitor under which the program is executed*: OS 360/50, WATFOR compiler

*Programming languages used*: FORTRAN IV

*High speed store required*: 7056 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 528

*Keywords descriptive of problem and method of solution*: Solid State, Symmetry, Band Structure, Group Theory.

*Nature of the physical problem*

The second section of a program to perform the symmetry part of band structure calculation. This part accepts the Luehrmann tables [1] as input and stores them in an appropriate manner permitting easy access to any element in the table.

*Method of solution*

Expansion of the wave function in terms of symmetrized plane waves.

*Restrictions on the complexity of the problem*

Limited to cubic lattices.

*Typical running time*

8-15 seconds.

*Reference*

[1] A. W. Luehrmann, Advan. Phys. 17 (1968) 65, 1.

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* Work supported by U.S. Air Force, Office of Scientific Research, grant number AFOSR 1709-69.

** Present address: Laboratoire de Spectrométrie Physique, CEDEX 53, 38-Grenoble-Gare, France.

*** Since the acceptance of this paper for publication Dr. O. Moller was tragically killed in an automobile accident.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 26-32. NORTH-HOLLAND PUBLISHING COMPANY

# SYMMETRY AND BAND STRUCTURE.
# III. CONSTRUCTION OF SYMMETRIZED HAMILTONIAN MATRIX *

V. HOFFSTEIN ** and O. MOLLER ***
*Physics Department, Polytechnic Institute of Brooklyn, Brooklyn, New York* 11201, *USA*

Received 12 October 1970

*Title of program* (32 characters maximum): SYMMETRY AND BAND STRUCTURE 3

*Catalogue number*: ACMF

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/50. *Installation*: Polytechnic Institute of Brooklyn

*Operating system or monitor under which the program is executed*: OS 360/50, WATFOR compiler

*Programming languages used*: FORTRAN IV

*High speed store required*: 8541 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 489

*Keywords descriptive of problem and method of solution*: Solid State, Band Structure, Symmetry, Group Theory, Symmetrized Plane Waves.

*CPC Library subprograms used*

*Catalogue number*: ACME *Title*: SYMMETRY AND BAND STRUCTURE 2 *Refs. in CPC*: 2 (1971) 17

*Nature of the physical problem*

The third section of a program to perform the symmetry part of band structure calculations. This part constructs symmetrized plane waves and evaluates matrix elements between them [1,2].

*Method of solution*

Expansion of the wave function in terms of symmetrized plane waves.

*Restrictions on the complexity of the problem*

Limited to cubic lattices.

*Typical running time*

15-30 seconds.

*References*

[1] A. W. Luehrmann, Advan. Phys. 17 (1968) 65, 1.
[2] V. Hoffstein and D. S. Boudreaux, Phys. Rev., to be published.

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* Work supported by U.S. Air Force, Office of Scientific Research, Grant Number 1709-69.

** Present address: Laboratoire de Spectrométrie Physique, CEDEX 53, 38-Grenoble-Gare, France.

*** Since the acceptance of this paper for publication Dr. O. Moller was tragically killed in an automobile accident.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 33-39. NORTH-HOLLAND PUBLISHING COMPANY

# ENERGY LEVEL CALCULATIONS IN DAVYDOV MODEL *

S. M. ABECASIS, F. R. FEMENIA
*Laboratorio de Radiaciones, IIAE, Buenos Aires, Argentina*

and

E. S. HERNANDEZ
*Facultad de Ciencias Exactas, Universidad Nacional de Buenos Aires, Argentina*

Received 20 April 1970
Revised manuscript received 18 May 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): Energy levels in Davydov model

*Catalogue number*: ABOE

*Computer for which the program is designed and others upon which it is operable*

*Computer*: Bull General Electric 625. *Installation*: Sistema de Computación de Datos, Yacimientos Petrolíferos Fiscales, Buenos Aires.

*Operating system or monitor under which the program is executed*: GECOS

*Programming languages used*: FORTRAN IV

*High speed store required*: 8 400 words. *No. of bits in word*: 36

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1326

*Keywords descriptive of problem and method of solution*: Nuclear, Excitation Energies, Energy Ratios, Davydov Model, Davydov-Chaban Model, Bessel Interpolation Formula, Newton-Raphson Method, Regula Falsi Method, Half-Interval Search, Gamma Function.

*Nature of physical problem*

The program is designed to calculate collective excitations and energy level ratios with the Davydov model [1] in terms of the three parameters $\alpha$, $\mu$ and $\gamma_0$.

*Method of solution*

Bessel formula is used to interpolate the energy levels predicted by the Davydov-Filippov model [2]. Newton-Raphson is applied to find the root of a fourth degree equation. A transcendental equation is solved either by the regula falsi or the half-interval search methods. The gamma function $\Gamma(x)$ is evaluated either with the Stirling series expansion or a seventh degree polynomial, according to the value of the argument (ref. [3]).

*Restrictions on the complexity of the problem*

This program can be used for a wide range of the parameters $\alpha$, $\mu$ and $\gamma_0$ fulfilling the conditions $8^\circ \leqslant \gamma_0 \leqslant 30^\circ$ and $0 \leqslant \mu \leqslant 1$. Computations are performed

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* Work done under the partial auspicies of the Consejo Nacional de Investigaciones Científicas y Técnicas and the Fundación Esso.

with the energy levels of the ground state rotational band from $I = 0$ up to 20 (by steps of 2) and those of the anomalous band for $I = 2$ up to 10 (by steps of 1) of the Davydov-Filippov model [4].

*Typical running time*

The test run for one nucleide takes about 8 minutes for compilation and 22 seconds for execution.

*Unusual features of the program*

Successive level sequences can be performed in the same run. Essentially the same algorithm described here may be used to search the best value for the model parameters.

This program allows one to compute energy levels and their ratios in the Davydov-Chaban model [5], with a minimum of alterations.

*References*

[1] A. S. Davydov, Nucl. Phys. 24 (1961) 682.
[2] A. S. Davydov and G. F. Filippov, Nucl. Phys. 8 (1958) 237.
[3] X. de Talance, Fonction gamma (Bull-General Electric, Bibliothèque Scientifique No. 00.05.006 F, 1966).
[4] R. B. Moore and W. White, Can. J. Phys. 38 (1969) 1149.
[5] A. S. Davydov and A. A. Chaban, Nucl. Phys. 20 (1960) 499.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 40-46. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTER-ASSISTED ANALYSIS OF GAMMA-RAY SPECTRA

G. D. ATKINSON Jr., J. B. WHITWORTH and S. J. GAGE
*Nuclear Reactor Laboratory, Department of Mechanical Engineering,*
*The University of Texas at Austin, Austin, Texas* 78712, *USA*

Received 20 October 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): NAA

*Catalogue number*: ABMB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: The University of Texas Computation Center, Austin, Texas 78712

*Operating system or monitor under which the program is executed*: UT1

*Programming languages used*: FORTRAN

*High speed store required*: $17\,000_8$ words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Disc

*No. of cards in combined program and test deck*: 1344

*Keywords descriptive of problem and method of solution*: Nuclear, Spectroscopy, Photopeak Identification, Qualitative Analysis, Gamma-Ray Spectra, Isotope, Lagrangian Interpolation.

*Nature of physical problem*

The program automatically analyzes multi-element gamma-ray spectra obtained with high resolution detectors. Peak energies and net areas are determined, and possible sources of individual gamma-rays are given.

*Method of solution*

Peaks are identified by slope changes in the spectrum. Peak statistics are determined by Covell's method [1], and peak identification is performed by table look-up.

*Restrictions on the complexity of the problem*

The gamma-ray spectra cannot contain more than 1024 channels, and the energy calibration curve must be a polynomial of degree 5 or less. The look-up table cannot contain more than 1000 gamma-ray energies, entered in ascending order.

*Typical running time*

To compile the program takes 5 seconds of central processor time. To run a typical 1024 channel spectrum takes 2-3 seconds.

*Unusual features of the program*

The NAA option to search a gamma-ray reference table simplifies multi-component trace element analysis. The short field length and running time allow rapid turn around in both batch processing and remote time sharing systems.

*Reference*

[1] D. F. Covell, Anal. Chem. 31 (1959) 1785.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 47-54. NORTH-HOLLAND PUBLISHING COMPANY

# TRANSPORT COLLISION INTEGRALS FOR A DILUTE GAS

H. O'HARA and F. J. SMITH

*Computer Laboratory and Computer Science Department, Queen's University, Belfast, Northern Ireland*

Received 5 May 1970
Revised manuscript received 16 October 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): TRANSPORT COLLISION INTEGRALS

*Catalogue number*: ACQN

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL 1907. *Installation*: Computer Laboratory, Queen's University, Belfast, N. Ireland

*Operating system or monitor under which the program is executed*: QUBE

*Programming languages used*: FORTRAN IV

*High speed store required*: 20 500 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1750

*Keywords descriptive of problem and method of solution*: Atomic, Molecular, Fluid Dynamics, Gas, Transport Property, Collision Integral, Impact Parameter, Clenshaw-Curtis, Potential, Orbiting, Lennard-Jones, Chebyshev

*Nature of physical problem*

The reduced collision integrals $\Omega^{(L,S)*}(T)$ are calculated to any desired relative accuracy. These integrals are used for the determination of the transport properties of dilute gases.

*Method of solution*

The reduced collision integrals can be expressed in the form of triple integrals which are evaluated using the Clenshaw-Curtis quadrature formula. This method is ideally suited to the automatic evaluation of definite integrals because of its accuracy and the possible error estimates available. Some of the integrals evaluated in the program contain singularities or they are badly behaved; these difficulties are overcome by using various changes of variable.

*Restrictions on the complexity of the problem*

The values of $L, S$ cannot exceed MAXL and MAXS respectively which are less than 6, and the number of reduced temperatures treated in one run cannot exceed 60. The program has been tested successfully for relative accuracies as small as 0.00001. The program is designed for any potential - specified in a function segment VF(R) which must be supplied by the user - which has an inner repulsive potential core and which falls to zero faster than $1/R^2$ for large $R$.

*Typical running time*

On our ICL 1907 (about the same speed as an IBM 7090) a set of transport properties at 40 different reduced temperatures and for $1 \leqslant L, S \leqslant 6$ can be calculated for the 12-6 potential to a relative accuracy 0.01 in 1 minute. For an accuracy 0.0001, 10 minutes are required.

*Unusual features of the program*

On machines with a floating point FORTRAN word length less than 48 bits the program should be run double length or failures may be flagged.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 55-58. NORTH-HOLLAND PUBLISHING COMPANY

# PRINTER-PLOTTER ROUTINE

C. Fred MOORE
*Center for Nuclear Studies, University of Texas, Austin, Texas 78712, USA*

Received 22 October 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): PLOTT

*Catalogue number*: ABOI

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: University of Texas

*Operating system or monitor under which the program is executed*: UT1

*Programming languages used*: FORTRAN IV

*High speed store required*: 1811 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card reader; Line printer

*No. of cards in combined program and test deck*: 446

*Keyword description of problem and method of solution*: General, Graphical Display, Printer Plotter

*Nature of physical problem*
The purpose of this subroutine is to obtain directly on a line printer a crude plot. The subroutine will plot any number of arrays on a surface of variable size limited only by the printer capacity. The subroutine run time is less than one second. The subroutine does not disturb the arrays being plotted.

*Method of solution*
The maximum and minimum values of each coordinate are found. The data are then modified by an appropriate transformation such that the values range from 0 to "NCL" for the horizontal coordinate and from 0 to "NLS" for the vertical coordinate. These are rounded and truncated into integer values. The integer values are then used to locate the Hollerith symbol in memory. If this location is already occupied by a symbol, an equal sign is substituted for the symbol. The entire Hollerith array then represents the plot itself and is consequently printed. The routine has been on the University of Texas systems tape library for four years [1].

*Restrictions on the complexity of the problem*
This routine may be used to plot linear, semi-log and semi-square-root graphs. The routine checks input for obvious errors and informs the user.

*Typical running time*
The typical running time is one second.

*Reference*

[1] C. Fred Moore, J5 UTEX PLOTT, Computation Center, University of Texas (1967).

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 59-78. NORTH-HOLLAND PUBLISHING COMPANY

# DERIVATION OF THE ORBIT OF A DOUBLE STAR FROM OBSERVATIONS MADE WITH AN INTENSITY INTERFEROMETER

D. HERBISON-EVANS
*School of Physics, Sydney University, Australia* 2006

Received 28 September 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): BIN DYN

*Catalogue number*: AACD

*Computer for which the program is designed and others upon which it is operable*

*Computer*: English Electric KDF9. *Installation*: Sydney University, Australia 2006

*Operating system or monitor under which the program is executed*: KIDSGROVE ALGOL COMPILER

*Programming languages used*: ALGOL, USERCODE

*High speed store required*: 25 000 words. *No. of bits in a word*: 48

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Printer; Paper Tape Reader; Paper Tape Punch

*No. of lines in combined program and test deck*: 500

*Keywords descriptive of problem and method of solution*: Astrophysics, Interferometer, Binary-star, Minimisation, Simplex Method.

*Nature of the physical problem*

The data from a stellar intensity interferometer [1] consists of a set of observations of the correlation of the light from two optical reflectors with a given separation (the baseline). If the star is double the data can be used to find the orbit of the double star. This has been done for the star $\alpha$ Virginis [2].

*Method of solution*

Using a test set of orbital parameters a simplex method [3] is used to minimize the weighted squares of the differences between the corresponding calculated and observed correlations.

*Restrictions on the complexity of the problem*

The program can cope with at most 819 observations made at up to 12 baselines, although this is easily altered. The stars are assumed to present uniform circular discs and not to eclipse. The reflectors are assumed to be negligibly small. The program uses only the first order Newton-Raphson solution for Kepler's equation.

*Typical running time*

On an English Electric KDF9 (about the speed of an IBM 7090) with 819 observations each residual takes about 5 seconds to calculate if a machine coded inner loop is used (otherwise 20 seconds). A full 11 parameter minimisation takes about 1 hour. The time is proportional to the number of observations.

*Unusual features of the program*

Two subprograms have been written in USERCODE (machine language). These can be replaced by their ALGOL equivalents.

*References*

[1] R. Hanbury Brown, J. Davis, L. R. Allen and J. M. Rome, Monthly Notices Roy. Astron. Soc. 137 (1967) 375.
[2] D. Herbison-Evans, R. Hanbury Brown, J. Davis and L. R. Allen, Monthly Notices Roy. Astron. Soc., to be published.
[3] J. A. Nelder and R. Mead, Computer J. 7 (1965) 308.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 79-86. NORTH-HOLLAND PUBLISHING COMPANY

# A PROCEDURE FOR NONLINEAR LEAST SQUARES REFINEMENT IN ADVERSE PRACTICAL CONDITIONS

J. LANG and R. MÜLLER

*Laboratorium für Kernphysik der Eidgenössischen Technischen Hochschule*, 8049 *Zürich*, *Switzerland*

Received 23 December 1970

## PROGRAM SUMMARY

*Title of program*: NONLINEAR LEAST SQUARES FIT

*Catalogue number*: ABGA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6400/6500. *Installation*: ETH

*Operating system or monitor under which the program is executed*: SCOPE 3.2, RUN-compiler

*Programming languages used*: FORTRAN IV

*High speed store required*: 7296 *words*. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card reader; Line printer

*No. of cards in combined program and test deck*: 465

*Keywords descriptive of problem and method of solution*: General, Nonlinear Least Squares Fit, Linearization Of Normal Equations, Iterative Solution.

*Nature of physical problem*

To determine optimum values of a set of parameters for the best agreement (in a least squares sense) between a given set of (experimental) values and corresponding calculated (theoretical) values where these values may be nonlinearly dependent on the parameters.

*Method of solution*

The minimum of the sum of the squared deviations of the experimental and theoretical values is found by iteration. The normal equations are linearized and transformed to the principal axis system. If in any iteration ill-conditioning yields a large correction of the parameters, the admissible variations are restricted to a hypercube with sides parallel to the principal axis [1].

*Typical running time*

2 seconds on the CDC 6400/6500 system for 6 parameters and 50 data points. The running time depends strongly, of course, on the number of parameters and measured points, the number of iterations needed and on how time consuming the evaluation of the function to be fitted is.

*Unusual features of the program*

None

*References*

[1] R. Deutsch, Estimation theory (Prentice-Hall, Englewood Cliffs, 1965) p. 101.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 87-93. NORTH-HOLLAND PUBLISHING COMPANY

# II. PROGRAM FOR CALCULATING TRIPLY DEGENERATE RAMAN BANDS OF SPHERICAL TOPS WITH AN ADAPTATION FOR INFRARED BANDS *

F. N. MASRI
*Department of Physics, University of Tennessee, Knoxville, Tennessee, USA*

and

I. R. WILLIAMS
*Knoxville College, Knoxville, Tennessee, USA*

Received 10 November 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): VIBROT II

*Catalogue number*: AAGE

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/65. *Installation*: University of Tennessee, Knoxville, Tennessee, USA

*Operating system or monitor under which the program is executed*: MVT-V18/HASP-II

*Programming languages used*: ALGOL

*High speed store required*: 6 000 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* IBM 2501 Card Reader; IBM 1403 Printer

*No. of cards in combined program and test deck*: 227

*Keywords descriptive of problem and method of solution*: Molecule, Raman, Scattering, Spectra, Spherical Tops, Coriolis Coupling.

*Nature of physical problem*

The program VIBROT II calculates the triply degenerate vibration-rotation bands of spherical top molecules in the gas-phase infrared or Raman spectrum. It is thus the analogue of the program VIBROT I [1] for symmetric top molecules and will be useful for band analysis in spherical tops in a corresponding way to VIBROT I for symmetric tops.

*Form of the program*

As with VIBROT I, the present program has a modular structure thus facilitating modifications of the procedures. The program has also been translated into FORTRAN IV.

*Restrictions on the complexity of the program*

Bands involved in accidental resonances and requiring a perturbation calculation may not be calculated with the program.

*Typical running time*

The test case requires 3 minutes 30 seconds to compile and run on the IBM 360/65 computer at the University of Tennessee.

*Reference*

[1] F. N. Masri and I. R. Williams, Computer Phys. Commun. 1 (1970) 349.

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* Supported in part by NASA Research Grant NGL 43-001-006.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 94-106. NORTH-HOLLAND PUBLISHING COMPANY

# DISTORTED WAVE BORN APPROXIMATION FOR NUCLEAR REACTIONS *

T. TAMURA, W. R. COKER and F. RYBICKI **
*Center for Nuclear Studies, University of Texas, Austin, Texas* 78712, *USA*

Received 21 September 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): DWBA-VENUS

*Catalogue number*: ABOH

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: University of Texas Computation Center

*Operating system or monitor under which the program is executed*: UT1

*Programming languages used*: FORTRAN IV

*High speed store required*: 44 208 words. *No. of bits in a word*: 60

*Is the program overlaid*? Yes

*No. of magnetic tapes required*: 4

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 4034

*Keywords descriptive of problem and method of solution*: Nuclear, Stripping and Pickup, Inelastic Scattering, Schrödinger Equation, Reaction, DWBA, Optical Model, Transition Amplitude, Spin-Orbit Coupling, Zero-range, Direct Interaction, Differential Cross Section, Particle-Gamma Correlation, Clebsch-Gordan Coefficient, Racah Coefficient, None-*j* Symbol, Statistical Tensors, Form Factor, Bound State, Collective Excitation, Spectroscopic Factor.

*Nature of physical problem*

The program DWBA-VENUS assembles the quantities needed to compute the transition amplitude for a given direct nuclear reaction in the distorted-wave Born approximation. The principal parts of the transition amplitude other than angular momentum and kinematic factors involve the radial wave functions of entrance and exit channels, obtained by solving the radial Schrödinger equation numerically with appropriate optical potentials including spin-orbit coupling; and, a form factor, either a single particle bound state radial wave function or a derivative of an optical potential. The bound state wave function is obtained by solving the radial Schrödinger equation for a state of given binding energy in a real Woods-Saxon potential with spin-orbit coupling.

*Method of solution*

The Störmer method [1] is used to solve the Schrödinger equation. The Störmer method with from two five points can be used. The method used to obtain the regular and irregular Coulomb functions is similar to that used by Buck et al. [2]. The various angular momentum coefficients required are evaluated from the exact analytic expressions [3]. The DWBA amplitude is evaluated in the form given by Satchler [4].

*Restrictions on the complexity of the problem*

The zero-range approximation is used, so that the cross sections are realistic only for inelastic scattering and for transfer reactions with light projectiles. The number of partial waves in a given channel is limited by dimension statements to 100. Also the product $(2s_a+1)(2s_b+1)(j+s_a+s_b+1)$ must be $\leqslant 55$, where $s_a$ and $s_b$ are the incident and exit projectile spins, and $j$ is the total angular momentum transfer.

*References*

[1] P. Henrici, Discrete variable methods in ordinary differential equations (Wiley, New York, 1962) ch. 6.
[2] B. Buck, R. N. Maddison and P. E. Hodgson, Phil. Mag. 5 (1960) 118.
[3] G Racah, Phys. Rev. 62 (1942) 438.
[4] G. R. Satchler, Nucl. Phys. 55 (1964) 1.

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* Work supported in part by the U.S. Atomic Energy Commission.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 107-113. NORTH-HOLLAND PUBLISHING COMPANY

# RELATIVISTIC SELF-CONSISTENT FIELD PROGRAM FOR ATOMS AND IONS

D. A. LIBERMAN and D. T. CROMER
*Los Alamos Scientific Laboratory,*
*Los Alamos, New Mexico, USA*

and

J. T. WABER
*Northwestern University, Evanston, Illinois, USA*

Received 7 October 1970

## PROGRAM SUMMARY

*Title of program*:(32 characters maximum): HEX

*Catalogue number*: AAKB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: Los Alamos Scientific Laboratory

*Operating system or monitor under which the program is executed*: SCOPE

*Programming languages used*: FORTRAN IV

*High speed store required*: 13 000 words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: 1

*What other peripherals are used*? Card reader; Card punch; Printer

*No. of cards in combined program and test deck*: 1333

*Keywords descriptive of problem and method of solution*: Atomic Structure, Self-Consistent Field, Dirac Equation, Hartree-Fock-Slater, Dirac-Slater.

*Nature of physical problem*

The program HEX performs self-consistent field calculations for atoms and ions using the Dirac operator in the one-electron equations [1]. The radial wavefunctions, charge density, potential function, total energy, and electron binding energies of an atom or ion are available as output.

*Method of solution*

The differential equations are solved by standard numerical methods. Self-consistency is obtained by iteration.

*Restrictions on the complexity of the problem*

There is provision for 35 shells in the program. Instabilities may prevent convergence in some cases.

*Typical running time*

On the CDC 6600 computer a few seconds to a few minutes are required in most cases.

*Unusual features in the program*

There is provision for several types of potential function. Electron binding energies may be computed without reference to Koopmans' theorem.

*Reference*

[1] D. A. Liberman, J. T. Waber and D. T. Cromer, Phys. Rev. 137 (1965) A27.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 114-123. NORTH-HOLLAND PUBLISHING COMPANY

# CLASSICAL RELATIVE MOTION OF 2 PARTICLES

D. BANKS, I. C. PERCIVAL and J. McB. WILSON
*Department of Physics, University of Stirling, Scotland*

Received 1 October 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): EVAR

*Catalogue number*: ACQT

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ELLIOT 4130. *Installation*: University of Stirling, Scotland

*Operating system or monitor under which the program is executed*: ENL 23

*Programming languages used*: FORTRAN

*High speed store required*: 20 000 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 3452

*Keywords descriptive of problem and method of solution*: Atomic, Molecular, Astrophysics, Classical, Coulomb, Diatomic, Euler, Forces, Frame, Gravitational, Hydrogen, Interatomic, Kepler, Newtonian, Orbit, Particle, Runge-Kutta, Scattering, State, Vibrational.

*Nature of the physical problem*

Flexible representation of the classical relative motion of two particles interacting through a general central force.

*Method of solution*

A general terminology of states and frames is introduced which allows changes from one state or frame to another to be defined. The frame changes are analytic. The state changes are made by solution of Newton's equations of motion using a fourth-order Runge-Kutta formula [1].

*Restrictions on the complexity of the problem*

Limited to central forces.

*Typical running time*

This depends on the form of the potential, the boundary conditions and the integration time specified.

*Reference*

[1] R. A. Buckingham, Numerical methods (Pitman, London, 1962).

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 127-138. NORTH-HOLLAND PUBLISHING COMPANY

# FOUR67, A FAST FOURIER TRANSFORM PACKAGE

J. P. CHRISTIANSEN
*UKAEA, Culham Laboratory, Abingdon, Berkshire, UK*

and

R. W. HOCKNEY
*University of Reading, Reading, Berkshire, UK*

Received 4 December 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): FOUR67

*Catalogue number*: ABUA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL KDF9. *Installation*: UKAEA Culham Laboratory

*Operating system or monitor under which the program is executed*: EGDON 3

*Programming languages used*: ASA FORTRAN

*High speed store required*: 2800 words. *No. of bits in a word*: 48

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer (for testing)

*No. of cards in combined program and test deck*: 1122

*Keywords descriptive of problem and method of solution*: Plasma Physics, M.H.D., Fluid Dynamics, Fast Fourier Transform, Fourier, Time Series Analysis, Analysis, Synthesis, Sine Analysis, Cosine Analysis, Harmonic.

*Nature of physical problem*

FOUR67 performs a finite Fourier analysis or synthesis on a given vector. It can carry out sine analysis or synthesis for odd functions, cosine analysis or synthesis for even functions, and sine and cosine analysis or synthesis for periodic functions. It was developed by one of the authors (RWH), a listing together with timing details for the CDC6600 and IBM 360/67 has previously been given [1]. The package has now been edited and documented (JPC) for publication.

*Method of solution*

It is known [2] that the harmonics in a finite Fourier expansion of a function $u(x)$ can be computed exactly from a discrete set of equidistantly spaced values $u(\Delta x)$, $u(2\Delta x)$, $u(3\Delta x)$ .... To minimize the number of arithmetic operations involved, FOUR67 employs a two-folding method [3] before multiplication with the sine or cosine terms. The two-folding method, which takes advantage of the symmetry of sine and cosine functions, implies additions only and is therefore well-suited to fast numerical computations.

*Restrictions on the complexity of the program*

FOUR67 will perform a finite Fourier analysis or synthesis (of any of the 3 types mentioned above), on any real vector with a dimension $N = 2^{\mathrm{IQ}} + 1$. The calculation is done in floating point form, the integer IQ is limited to 3 at the lower end by the logic, and at the upper end only by limitations of storage.

*Typical running time*

The execution times depend on $N$ as well as on the type of analysis or synthesis. On the ICL KDF9 a vector of length 64 + 1 takes approximately 0.2 sec to analyse or synthesise. Timing details for the CDC6600 and IBM 360/67 have been given in ref. [1].

*Unusual features of the program*

The program is written in ASA FORTRAN apart from the use of symbolic dimensions, which on certain computer systems must be replaced by actual numerical values. The PRELUDE section should then be removed. When used repeatedly this package should be programmed in assembly code to achieve maximum speed, and FOUR67 has been designed with this end in mind.

*References*

[1] R. W. Hockney, in: Methods in computational physics, Vol. 9, eds. B. Alder and S. Fernbach (Academic Press, New York, 1970) p. 135.
[2] E. T. Whittaker and G. Robinson, The calculus of observations (Blackie, Glasgow, 1944) p. 260.
[3] R. W. Hockney, SU-IPR-53, Stanford University (1966).

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 139-155. NORTH-HOLLAND PUBLISHING COMPANY

# DELSQPHI, A TWO-DIMENSIONAL POISSON-SOLVER PROGRAM

J. P. CHRISTIANSEN
*UKAEA, Culham Laboratory, Abingdon, Berkshire, UK*
and
R. W. HOCKNEY
*University of Reading, Reading, Berkshire, UK*

Received 4 December 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): DELSQPHI

*Catalogue number*: ABUB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL KDF9. *Installation*: UKAEA, Culham Laboratory

*Operating system or monitor under which the program is executed*: EGDON 3

*Programming languages used*: ASA FORTRAN

*High speed store required*: 5200 words. *No. of bits in a word*: 48

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Line Printer (for test only)

*No. of cards in combined program and test deck*: 1630

*CPC Library subprograms used*

*Catalogue number*: ABUA; *Title*: FOUR67; *Ref. in CPC*: 2 (1971) 127.

*Keywords descriptive of problem and method of solution*: Plasma Physics, M.H.D., Fluid Dynamics, Poisson, Fast Fourier Transform, Recursive Cyclic Reduction, Two-dimensional.

*Nature of physical problem*

Plasma simulations, fluid flow problems and many related computations require a fast method of solving Poisson's equation on a discrete mesh. DELSQPHI has been written for this purpose: it is an edited ASA FORTRAN version of the POT1 package written by one of the authors (RWH) and previously described elsewhere [1].

*Method of solution*

The solution of Poisson's equation is obtained using a 5-point finite difference approximation. The method of solution is "direct", i.e. it does not involve any iterative procedures. A reduction of the matrix equations eliminates the unknown quantities on alternate lines, ("odd lines") and a fast Fourier transform technique [1,2] is used to decouple the remaining equations. The FOUR67 package is used for this [2]. The Fourier components of the potential are found by a method called recursive cyclic reduction [3]. The inverse Fourier transform [2] yields the solution on even lines and the use of the 5-point approximation completes the solution for the odd lines. For storage economy the calculated potential overwrites the charge distribution which was previously supplied as input.

*Restrictions on the complexity of the program*

DELSQPHI will accept any real charge distribution specified in floating point form on a rectangular mesh of dimensions NX and NY. The maximum size of the mesh is determined by the size of the core store of the computer employed.

*Typical running time*

The execution times depend on the mesh dimensions [3] and on the set of boundary conditions chosen. On the ICL KDF9 at Culham Laboratory the solution is obtained over a 64 × 64 mesh in 13 sec when the electric field is zero on the $(x, y)$ boundaries, and in 10 sec when the potential is periodic in $(x, y)$. Compilation and loading on the KDF9 take about 250 sec.

*Unusual features of the program*

The program is written in ASA FORTRAN apart from the use of symbolic dimensions, which on certain computer systems must be replaced by actual numerical values. The PRELUDE section should then be removed.

*References*

[1] R. W. Hockney, in: Methods in computational physics, Vol. 9, eds. B. Alder and S. Fernbach (Academic Press, New York, 1970) p. 135.
[2] J. P. Christiansen and R. W. Hockney, Computer Phys. Commun. 2 (1971) 127.
[3] R. W. Hockney, J. Assoc. Computing Machinery 12 (1965) 95.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 157-167. NORTH-HOLLAND PUBLISHING COMPANY

# SOLUTION OF POISSON'S EQUATION IN CYLINDRICAL COORDINATES

M. H. HUGHES
*UKAEA, Culham Laboratory, Abingdon, Berkshire, UK*

Received 4 December 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): DELSQRZ

*Catalogue number*: ABUC

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL KDF9. *Installation*: UKAEA, Culham Laboratory

*Operating system or monitor under which the program is executed*: Egdon 3

*Programming languages used*: ASA FORTRAN

*High speed store required*: 5K words. *No. of bits in a word*: 48

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Line Printer (for test only)

*No. of cards in combined program and test deck*: 1131

*CPC Library subprograms used*

*Catalogue number*: ABUA; *Title*: FOUR67; *Ref. in CPC*: 2 (1971) 127.

*Keywords descriptive of problem and method of solution*: Plasma Physics, M.H.D., Fluid Dynamics, Poisson, Cylindrical, Fast Fourier Tranform.

*Nature of the physical problem*

The DELSQRZ package obtains a rapid solution of Poisson's equation in the $(r, z)$ plane subject to the following boundary conditions:

1. The potentials on the axis and at some radius $r = r_0$ are *always* given;
2. Either (i) the potential is given on the $z$-boundaries, or (ii) periodic $z$-geometry.

*Method of solution*

Poisson's equation is replaced by a 5-point finite difference approximation and the resulting equations are solved by a method based on Fourier analysis [1-3]. The FOUR67 package is used for this [4].

*Restrictions on the complexity of the problem*

The $(r, z)$ plane is divided into a uniform rectangular mesh of dimensions NR and NZ (not necessarily equal). To simplify the Fourier analysis NZ is restricted to be a power of two.

*Typical running time*

On the Culham KDF9 loading and compilation takes 250 sec. The running time depends on the mesh size and on the $z$-boundary conditions. Typically, on a 64 × 64 mesh the times are 20 sec when the potential is given on the $z$-boundaries, and 15 sec when the $z$-geometry is periodic.

*Unusual features of the program*

The program is written in ASA FORTRAN apart from the use of symbolic dimensions, which on certain computer systems must be replaced by actual numerical values. The PRELUDE section should then be removed.

*References*

[1] R. W. Hockney, J. Assoc. Computing Machinery 12 (1965) 95.
[2] R. W. Hockney, A.P.S. Topical Conf. on Numerical Simulation of Plasmas, Los Alamos (1968).
[3] R. W. Hockney, in: Methods of computational physics, Vol. 9, eds. B. Alder and S. Fernbach (Academic Press, New York, 1970) p. 135.
[4] J. P. Christiansen and R. W. Hockney, Computer Phys. Commun. 2 (1971) 127.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 168-172. NORTH-HOLLAND PUBLISHING COMPANY

# CODNUM, A PROGRAM TO CHANGE THE PUNCHING CODE AND TO NUMBER A DECK OF CARDS *

F. R. FEMENIA

*Laboratorio de Radiaciones, IIAE, Facultad de Ciencias Exactas, Perú* 272, *Buenos Aires, Argentina*

Received 19 May 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): CODNUM

*Catalogue number*: ACQU

*Computer for which the program is designed and others upon which it is operable*

*Computer*: Bull General Electric 625. *Installation*: Sistema de Computación de Datos, Yacimientos Petrolíferos Fiscales, Buenos Aires.

*Operating system or monitor under which the program is executed*: GECOS

*Programming languages used*: FORTRAN IV

*High speed store required*: 500 words. *No. of bits in a word*: 36

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer; Card Punch

*No. of cards in combined program and test deck*: 291

*Keywords descriptive of problem and method of solution*: Character Code, Numeration, Number of Digits

*Nature of the problem*

CODNUM is a routine to change the code of a given set of characters punching a new deck in a desired code. A consecutive numeration is provided in the last four columns of each card, as well.

*Method of solution*

The card is read as alphanumeric data into an array and every character punched in columns 7 through 72 is tested looking for differences in code. These are corrected and the content of the array thus modified along with the numeration is punched in a new card.

*Restrictions on the complexity of the problem*

The present version is designed to change BULL-GE and IBM 026 characters which differ from IBM 029 code. To adapt it to another installation, some minor changes in code and logic will be necessary.

*Typical running time*

In the Bull-Ge 625 computer CODNUM took 44 seconds for compilation and the complete processing of 900 cards was performed in 43 seconds.

*Unusual features of the program*

Modified versions of the program that only copy the card and punch the number and/or skip the code checking for comment cards, can easily be obtained.

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* Work done under the partial auspices of the Consejo Nacional de Investigaciones Científicas y Técnicas and the Fundación ESSO.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 173-174. NORTH-HOLLAND PUBLISHING COMPANY

# ERRATUM NOTICES

*Title of manuscript*: A program to calculate a general recoupling coefficient
*Author*: P. G. Burke
*Reference*: Computer Physics Communications 1 (1970) 241
*Title of program*: NJSYM
*Catalogue number*: AAGD

* * *

*Title of manuscript*: Transport collision integrals for a dilute gas
*Authors*: H. O'Hara and F. J. Smith
*Reference*: Computer Physics Communications 2 (1971) 47
*Title of program*: TRANSPORT COLLISION INTEGRALS
*Catalogue number*: ACQN

*Title of manuscript*: Angular momentum coupling coefficients
*Author*: T. Tamura
*Reference*: Computer Physics Communications 1 (1970) 337
*Title of program*: GEOMETRICAL COEFFICIENT
*Catalogue number*: ABMA

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 175-179. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR CALCULATING RELATIVISTIC ELASTIC ELECTRON-ATOM COLLISION DATA

A. C. YATES

*Department of Chemistry, Indiana University, Bloomington, Indiana* 47401, *USA*

Received 19 March 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): A SCAT

*Catalogue number*: ACQX

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: Indiana University Research Computing Center, Bloomington, Indiana

*Operating system under which the program is executed*: SCOPE 3.3

*Programming languages used*: FORTRAN IV

*High speed store required*: 19 020 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 635

*Keywords descriptive of problem and method of solution*: Atomic, Scattering, Electrons, Relativistic, Partial-Waves, Spin Polarization, Numerov.

*Nature of physical problem*

The program calculates angular distributions (differential cross sections) and spin-polarization distributions of electrons scattered elastically by atomic targets within the framework of the static field approximation, by solving the radial Dirac equations.

*Method of solution*

The radial Dirac equations are cast into Schrödinger form, and the resulting second-order differential equation is solved by using the modified form of the Numerov algorithm. The partial-wave series are then summed directly.

*Restrictions on the complexity of the problem*

As written, the program handles any scalar potential written as a sum of Yukawa terms, but is easily modified to treat other functional forms, or numerical tables.

*Typical running time*

The test run for $Z = 7$, at 500 eV required 25 partial waves and takes 17 seconds to execute on the CDC 6600.

*References*

[1] A. C. Yates and T. G. Strand, Phys. Rev. 170 (1968) 184.
[2] A. C. Yates, Phys. Rev. Letters 20 (1968) 829.
[3] A. C. Yates and R. A. Bonham, J. Chem. Phys. 50 (1969) 1056.
[4] A. C. Yates and M. Fink, Phys. Rev. Letters 22 (1969) 1.
[5] A. C. Yates, Phys. Rev. 176 (1968) 173.
[6] M. Fink and A. C. Yates, Atomic Data 1 (1970) 385.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 180-190. NORTH-HOLLAND PUBLISHING COMPANY

# A NEW VERSION OF A GENERAL PROGRAM TO CALCULATE ANGULAR MOMENTUM INTEGRALS IN ATOMIC STRUCTURE

A. HIBBERT
*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, Northern Ireland*

Received 10 March 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): WEIGHTS NEW VERSION

*Catalogue number*: ACQV

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL 1907. *Installation*: Queen's University, Belfast, Northern Ireland

*Operating system or monitor under which the program is executed*: QUBE

*Programming language used*: FORTRAN IV

*High speed storage required*: 28 K words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer; Card Punch (Optional)

*No. of cards in combined program and test deck*: 2572

*CPC Library subprograms used*

| *Catalogue numbers* | *Titles* | *Refs. in CPC* |
|---|---|---|
| ACQB | P SHELL C.F.P. | 1 (1969) 15 |
| ACQC | D SHELL C.F.P. | 1 (1969) 16 |
| AAGD | NJSYM | 1 (1970) 241 |
| AAGD0001 | ADAPT NJSYM FOR WEIGHTS | 2 (1971) 180 |

*Reference to other published version of this program*

*Catalogue number*: ACQL; *Title*: WEIGHTS; *Ref. in CPC*: 1 (1970) 359.

*Keywords descriptive of problem and method of solution*: Atomic, Configuration Interaction, Racah, Coefficients Of Fractional Parentage, Recoupling Coefficients, Slater Integrals, Average Energy, Complex Atoms, Wave Function, Bound States, *LS* Coupling.

## ADAPTATION SUMMARY

*Title of manuscript*: Adaptation of NJSYM and GENSUM for use with Program WEIGHTS

*Adaptor's name and address*: A. Hibbert, Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Northern Ireland.

*Title of adaptation*: ADAPT NJSYM FOR WEIGHTS

*Adaptation number*: 0001

*Reference to original program*: *Catalogue number*: AAGD; *Title*: NJSYM; *Ref. in CPC*: 1 (1969) 241, 2 (1971) 173

*Author of original program*: P. G. Burke

*No. of cards required to effect adaptation* (including directive cards): 4

*Nature of physical problem*

The purpose of the program is to express the matrix elements of the two-electron interaction of the hamiltonian as a weighted sum of radial Slater integrals.

*Method of solution*

The main difference between this code and the earlier version [1] is that the present code makes use of average energy expressions [2] where possible.

*Typical running time*

The six sets of configurations in the test data took 111 seconds on an ICL 1907. This should be compared with the time of 75 seconds for the first two sets of configurations, using the earlier version. The use of average energy contributions provides a varied improvement in time, but typically is of the order of 30%. Another factor which affects the comparison between these two times is a new compiler on our ICL 1907. This too reduces the execution time. The new compiler also appears to reduce the store required for programs of this sort of size by approximately 10%. Thus, the reduction in core storage from 30 K to 28 K is a result of the introduction of the new compiler, and the removal of four COMMON blocks (about 2 K words), balanced by 500 extra cards.

*References*

[1] A. Hibbert, Computer Phys. Commun. 1 (1970) 359.
[2] J. C. Slater, Quantum theory of atomic structure, Vol. 1 (McGraw-Hill, New York, 1960).

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 191-200. NORTH-HOLLAND PUBLISHING COMPANY

# LANTHANIDE CRYSTAL FIELD FITTING ROUTINE

G. E. STEDMAN *
*Department of Physics, Queen Mary College, Mile End Road, London E.1, UK*

Received 1 January 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): CRYSTAL FIELD AND G VALUE

*Catalogue number*: ACAB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: ICL 1905E. *Installation*: Queen Mary College, Mile End Road, London E.1

*Operating system or monitor under which the program is executed*: George 2E

*Programming languages used*: FORTRAN IV

*High speed store required*: 24-32 K words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? None

*No. of cards in combined program and test deck*: 1588

*Keywords descriptive of problem and method of solution*: Solid State, Crystal Field Parameters, Energy Level Fitting, *g* Values, Least Squares Nonlinear Parameter Estimation, Paramagnetic Ions, Lanthanide Spectra.

*Nature of physical problem*

The electronic states of paramagnetic ions in crystals are split by the electric field from other ions. These splittings may be fitted by a suitable choice of crystal field parameters $A_n^m\langle r^n\rangle$. The routine performs this fit and outputs a comparison of experimental and theoretical energies, and also (as required) *g*-values and wavefunctions for the crystal field states.

*Method of solution*

The calculation of energies from crystal field parameters requires matrix diagonalisations. The parameters are adjusted under the control of an efficient fitting procedure [1] to give a least squares fit to the experimental energies. The derivatives required are computed from the eigenvectors obtained in the diagonalisation.

*Restrictions on the complexity of the program*

The routine is useful for lanthanides only.

*J*-mixing is neglected (cf. unusual features).

As written, each crystal field parameter is varied independently. However, one subroutine is easily modified so that $A_n^m/A_n^0$ is held constant provided $m > 0$.

The assignments of states within a manifold may not be taken into account during a fitting, though they may be checked afterwards.

*Typical running time*

For the test case (14 parameters, 2 manifolds, *J*-values 7.5 and 6.5, and non-zero imaginary parts to the matrix elements) the storage used is 24.8 K and the running time is approximately 80 sec per iteration, or 30 sec per function evaluation.

*Unusual features of the program*

The neglect of "*J*-mixing" (the coupling of the atomic manifolds by the crystal field) has many advantages, such as the possibility of using operator equivalents.

The program takes full advantage of block diagonalisations consequent on the particular site symmetry, with other similar economies.

*Reference*

[1] R. Fletcher and M. J. D. Powell, The Computer J. 6 (1963) 163.

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* Present address: Department of Physics, University of Canterbury, Christchurch, New Zealand.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 201-206. NORTH-HOLLAND PUBLISHING COMPANY

# HIGH SPEED EVALUATION OF $F_0(x)$ *

L. L. SHIPMAN and R. E. CHRISTOFFERSEN
*Department of Chemistry, University of Kansas, Lawrence, Kansas* 66044, *USA*

Received 8 October 1970
Revised manuscript received 23 March 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): DFZERO

*Catalogue number*: ACAA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: GE-635. *Installation*: University of Kansas

*Computer*: IBM 360/50. *Installation*: The Upjohn Company, Kalamazoo, Michigan, USA

*Computer*: CDC 3300. *Installation*: University of Mainz, Mainz, Germany

*Operating system or monitor under which the program is executed*: GECOS III

*Programming languages used*: FORTRAN IV

*High speed store required*: 634 words. *No. of bits in a word*: 36

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 286

*Keywords descriptive of the problem and method of solution*: Quantum Chemistry, Molecular Integral, Gaussian Orbital, 1s-Type Orbital, Integral Evaluation, Electronic Energy, Chebyshev Series, Asymptotic Expansion.

*Nature of the physical problem*

Much physical insight into the fundamental nature of molecules arises directly and indirectly from the calculation of the electronic energy. However, the ease of evaluating the various integrals that arise in the calculation of the electronic energy is strongly basis set dependent. The use of spherical gaussian basis orbitals allows major simplifications to occur in the integral evaluations, for all of the integrals that are required can be evaluated analytically, and require only the auxiliary function,

$$F_0(x) = \int_0^1 \exp[-xu^2]du ,$$

with $x \geqslant 0$. Consequently, efficient and accurate evaluation of $F_0(x)$ is essential, if practical procedures for energy evaluation are to be developed.

*Method of solution*

The argument range $0 \leqslant x$ is divided up into four intervals; $0 \leqslant x < 6.125$, $6.125 \leqslant x < 14$, $14 \leqslant x < 28$, and $28 \leqslant x$. In the first three intervals an eight-term, rearranged Chebyshev series (power series) is used to approximate $F_0(x)$. In the last interval an asymptotic approximation is used to evaluate $F_0(x)$.

*Restrictions on the complexity of the problem*

The relative error is less than $4 \times 10^{-13}$. DFZERO would not be useful for calculations in which a greater degree of accuracy is desired. Also DFZERO evaluates $F_0(x)$ for only positive or zero arguments.

*Unusual features of the program*

Speed in evaluation is coupled with a compact high speed store requirement. Rearranged Chebyshev series coefficients are introduced in DATA statements, so there is no overhead time required for their calculation before DFZERO can be called.

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* This work was supported in part by a grant from The Upjohn Company, Kalamazoo, Michigan, and a grant from the University of Kansas.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 207-213. NORTH-HOLLAND PUBLISHING COMPANY

# THE EVALUATION OF THE VOLUME OF THE PHASE SPACE OF *N* PARTICLES

K. KAJANTIE
*Department of Physics, University of Helsinki, Helsinki, Finland*
and
V. KARIMÄKI
*Department of Nuclear Physics, University of Helsinki, Helsinki, Finland*

Received 8 December 1970

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): RN

*Catalogue number*: AAUB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: Burroughs 6500. *Installation*: University of Helsinki

*Operating system or monitor under which the program is executed*: Unspecified

*Programming languages used*: FORTRAN IV

*High speed store required*: 917 words. *No. of bits in a word*: 48

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 300

*Keywords descriptive of problem and method of solution*: Nuclear, High Energy, Multiparticle Production, Phase Space, Statistical Model, Central Limit Theorem, Method Of Steepest Descent.

*Nature of physical problem*

In multiparticle production reactions of large multiplicity, $n$, a rough approximation to reality is to assume that the reaction probability is proportional to the volume of the phase space. At lower multiplicities the situation is complicated by the limitations in transverse momenta and by other more detailed dynamical effects. Similar remarks apply to the calculation of all quantities expressible in terms of phase space volumes: mass spectra, one-particle spectra, etc. The phase space distribution gives a kind of background to these, which then is modified by dynamical effects.

*Method of solution*

An approximation based on the saddle point method [1-3] is used.

*Restrictions on the complexity of the program*

The total multiplicity $n$ is taken to be less than 100, but this limit is easy to change.

*Typical running time*

For $n \approx 10$, the time needed to calculate one value of the phase space integral is about 0.1 sec for computers like CDC 6500 or Burroughs 6500.

*References*

[1] V.A. Kolkunov, JETP 43 (1962) 1448; English translation: Soviet Phys. JETP 16 (1963) 1025.
[2] F. Lurçat and P. Mazur, Nuovo Cimento 31 (1964) 140.
[3] G.H. Campbell, J.V. Lepore and R.J. Riddell Jr., J. Math. Phys. 8 (1967) 687.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 214-222. NORTH-HOLLAND PUBLISHING COMPANY

# RAPID EVALUATION OF FOUR-BODY CLUSTER CONTRIBUTIONS

G. P. MUELLER
*Code 7660, Naval Research Laboratory, Washington, D.C. 20390, USA*

Received 9 February 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): FOURBODY

*Catalogue number*: ABIA

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 3800. *Installation*: Naval Research Laboratory, Washington, D.C. 20390

*Operating system or monitor under which the program is executed*: SCOPE

*Programming languages used*: FORTRAN

*High speed store required*: 3 789 words. *No. of bits in a word*: 48

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 467

*Keywords descriptive of problem and method of solution*: Nuclear, Cluster Expansion, Numerical Integration, Four-Body Contributions, Haselgrove, Alpha Matter, Monte-Carlo, Equidistributed Sequence.

*Nature of physical problem*

Within the framework of the cluster expansion formalism we present a method for rapidly evaluating the four-body contributions to the ground state energy of an extended system of bosons, specifically, alpha matter. Since the numerical results for alpha matter have been published elsewhere [1], we present here a fictitious example for which the exact results are obtainable.

*Method of solution*

These calculations involve the numerical integration of six-dimensional integrals, which we evaluate using a method due to Haselgrove [2]. For the same accuracy, this method seems to require less running time and is easier to program than more conventional methods.

*Restrictions on the complexity of the problem*

The program is restricted to the evaluation of six-dimensional integrals, but can easily be modified to evaluate an integral of almost any dimension.

*Typical running time*

Approximately 15 seconds are needed on the CDC 3800 for results that are accurate to 5% for the example given here. For a more realistic problem, perhaps twice that much running time would be needed.

*References*

[1] G. P. Mueller and J. W. Clark, Nucl. Phys. A155 (1970) 561.
[2] C. B. Haselgrove, Math. Computation 15 (1961) 323.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 223-230. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM TO CALCULATE COMPLEX PHASE SHIFTS AND MIXING PARAMETERS OF ELASTIC SCATTERING OF SPIN $\frac{1}{2}$ PARTICLES ON SPIN $\frac{1}{2}$ TARGETS

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*Physikalisches Institut der Universität Erlangen, Glückstrasse 6, D852 Erlangen, Germany*

Received 16 February 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): PHASESHIFT ANALYSIS

*Catalogue number*: ABGB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 3300. *Installation*: Rechenzentrum der Universität Erlangen-Nürnberg, Erlangen

*Operating system or monitor under which the program is executed*: MASTER

*Programming languages used*: FORTRAN IV

*High speed store required*: 62387 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1796

*Keywords descriptive of problem and method of solution*: Nuclear, Density Matrix, Cross Section, Polarization, $S$-Matrix, Phase Shifts, Chi-Squared, Gaussian Normal Equations.

*Nature of physical problem*

For elastic scattering the differential cross section and the polarization are determined by the elements of the $S$-matrix. The $S$-matrix can be parametrized in terms of complex phases. Generally the complex phases are slowly varying functions of energy. Only when near resonances will the phases, corresponding to the spin and parity of the special resonance, show specific anomalies, which sometimes allow the determination of spin and parity of the resonance.

*Method of solution*

The complex phases and mixing parameters are obtained by a least squares fit of the differential cross section and polarization data. The minimization is performed iteratively by solving gaussian normal equations [1].

*Restrictions on complexity of the problem*

The program is such, that all complex phases up to $l = 3$ (one singlet and three triplets) and the singlet and one triplet for $l = 4$ can be calculated. Moreover all mixing parameters up to $\epsilon^{4+}$ can be computed. Until now, only analyses with angular momenta up to $l = 2$ were performed with this program. If the program is used to fit data with nonvanishing phase shifts for $l = 3$ and $l = 4$, it is necessary to increase the dimension of PKOEF and its corresponding quantum number arrays. The reason is that in this case "TENMO" [2] calculates more coefficients.

*Typical running time*

About two minutes for one iteration step.

*Unusual features of the program*

In order to calculate the gaussian normal equations it is necessary to break up a Taylor series of $Q$ (see below) at the linear limb. Therefore the calculated change of the parameters may not run to a minimum, but may run into the opposite direction or even exceed the minimum. If this happens, a step change is necessary. The program goes to $\frac{1}{33}$ of the original change. If this is not sufficient it bisects these values and, if necessary, changes the direction. The last two steps are iterated as long as the new $Q$ is better than the old one. Sometimes it may be more efficient to have other step changes. For this purpose the program has to be altered directly (see comment in program).

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* Present address: Max-Planck-Institut für Kernphysik, Heidelberg, Germany.

*References*

[1] Van der Waerden, Mathematische Statistik (Springer, Berlin, 1965).

[2] R. D. McCulloch, H. W. Graben, S. T. Thornton and H. B. Willard, Oak Ridge National Laboratory, Report 4121.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 231-237. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTATION OF BRODY-MOSHINSKY BRACKETS

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and
J. P. JEUKENNE
*Theoretical Nuclear Physics, University of Liège, Sart Tilman, 4000 Liège 1, Belgium*

Received 10 February 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): BRODY-MOSHINSKY BRACKETS

*Catalogue number*: ABGC

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/65. *Installation*: University of Liège

*Operating system or monitor under which the program is executed*: CS 360

*Programming languages used*: FORTRAN IV(G)

*High speed store required*: 8130 words. *No. of bits in a word*: 64

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 579

*CPC Library subprograms used*
*Catalogue number*: ABMA; *Title*: RACAH; *Ref. in CPC*: 1 (1970) 337

*Keywords descriptive of problem and method of solution*: Nuclear, Nuclear Spectra, Nuclear Structure, Two-Body Operator Matrix Elements, Hartree-Fock Calculations, Brody-Moshinsky Brackets.

*Nature of the physical problem*

The program computes the Brody-Moshinsky brackets $\langle nl, NL, \lambda | n_1 l_1, n_2 l_2, \lambda \rangle$ defined in refs. [1,2] and appearing in the calculation of matrix elements of two-body operators, when the single particle radial wave functions are those of a harmonic oscillator. Such matrix elements are encountered in shell-model and Hartree-Fock calculations.

*Method of solution*

A recursion relation [2] connecting Brody-Moshinsky brackets (B.M.B.) with increasing $n_1, n_2$ indices is used. The structure of the program is such that a minimum size core is needed to calculate the B.M.B.

*Restrictions on the complexity of the problem*

In the present form of the program, restrictions come only from the allowed dimensions which are sufficient for values of the indices $n_1, n_2 \leq 5$. For higher values of the indices, these dimensions may easily be increased, so that the size restrictions depend only on the computer storage available.

*Typical running time*

The running time is 0.40 sec for indices $n_1, n_2$ equal to 0,1 on the IBM 360/65 computer at the University of Liège.

*References*

[1] M. Moshinsky, Nucl. Phys. 13 (1959) 104.
[2] T. A. Brody and M. Moshinsky, Tables of transformation brackets (Gordon and Breach, London, 1967).
[3] T. Tamura, Computer Phys. Commun. 1 (1970) 337.

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* Chercheur I.I.S.N., on leave from the University of Liège, Belgium.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 239-260. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR ATOMIC WAVEFUNCTION COMPUTATIONS BY THE PARAMETRIC POTENTIAL METHOD

M. KLAPISCH *
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Received 6 January 1971

## PROGRAM SUMMARY

*Title of program*: MAPPAC

*Catalogue number*: AAKC

*Computer for which the program is designed and others upon which it is operable*

*Computer*: UNIVAC 1108; *Installation*: Orsay, France;
C.D.C.6600. Jerusalem, Israel.

*Programming language used*: FORTRAN IV

*High speed storage required*: 50 000 words of 36 bits

*Is the program overlaid?* No

*Number of magnetic tapes*: None

*What other peripherals are used?*: Card Reader; Printer; Punch.

*Number of cards in combined program and test deck*: 3600

*Keywords*: Atomic, Radial Wavefunctions, Central Field, Transition Probability, Spin-Orbit Coupling, Hyperfine Structure Fitting, Spectroscopy, Quality Criteria

*Nature of physical problem*

MAPPAC computes atomic radial wavefunctions, and many related quantities, such as Slater integrals, spin-orbit coupling, mixing of configurations, hyperfine structure, transition probabilities etc., in the framework of first-order perturbation theory, built upon an optimized central field [1-3].

*Method of solution*

The central field is represented by an analytical expression in which some parameters are free. Given initial values of these, an iterative computation is performed, which optimizes the central field according to one of the following quality criteria (available as input options)

(a) minimization of the r.m.s. deviation of the energy between theory and experiment ("spectroscopic criterion");

(b) minimization of the sum of total energies ("variational criterion");

(c) minimization of the perturbing operator ("perturbational criterion").

*Restriction on the complexity of the problem*

Wavefunctions are not relativistic, although first-order corrections to energies are computed.

Continuum wavefunctions are not computed.

Angular coefficients of integrals for open shells must be given as input (to obtain these, see for instance [4]).

Maximum number of wavefunctions: 30; of matrices: 30; maximum rank: 30; number of integrals: 300. Kinds of integrals programmed: 17. Number of levels to be computed at a time: 200.

Any atom or ion can be studied, except for those involving g-wave and higher wave electron orbitals.

*Unusual features of the program*

(a) On the physical aspect: the convergence of radial equations has been achieved in such a way that estimates of one electron energy parameters, or screening constants etc., are *not* required.

(b) On the preparation of data input: it has been made easy by thorough use of alphabetic symbols in data, and checking punching errors as far as possible.

*References*

[1] M. Klapisch, Thesis, Orsay (1969).
[2] S. Feneuille, M. Klapisch, E. Koenig and S. Liberman, Physica 48 (1970) 571.
[3] M. Aymar, M. Crange and M. Klapisch, J. Phys. (Paris) 31 (1970) suppl. C4, 141.
[4] A. Hibbert, Computer Phys. Commun. 1 (1970) 359.

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* Present address: Theoretical Physics Department, Hebrew University, Jerusalem, Israel.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 261-271. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR CALCULATING THE STATIC INTERACTION POTENTIAL BETWEEN AN ELECTRON AND A DIATOMIC MOLECULE

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*Greenbelt, Maryland* 20771, *USA*

A. L. V. TENCH
*Theoretical Physics Division, Atomic Energy Research Establishment, Harwell, Didcot, Berkshire, UK*

Received 16 March 1971
Revised manuscript received 7 May 1971

## PROGRAM SUMMARY

*Title of program*: STATIC INTERACTION POTENTIAL

*Catalogue number*: ACQW

*Computer*: IBM 360/75. *Installation*: A.E.R.E. Harwell

*Operating system or monitor under which the program is executed*: HASP MFT2

*Programming languages used*: FORTRAN IV

*High speed store required*: 52K words. *No. of bits in a word*: 32

*Is the program overlaid*? Yes

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card reader; Line printer; Disc IBM 2311; Data cell IBM 2314

*Number of cards in combined program and test deck*: 1800

*Keywords descriptive of problem and method of solution*: Quantum Chemistry, Molecular, Wavefunction, Single-Centre Expansion, Static Potential, Dipole Moment, Quadrupole Moment, Clebsch-Gordan Coefficient

*Nature of the physical problem*

This program calculates the single centre multipole expansion of the static potential for a diatomic molecule. It also calculates the dipole and quadrupole moments. It provides wavefunctions and the static potential in a form suitable for use in the companion program by Sinfailam [1].

*Method of solution*

The molecular orbitals are assumed to be given by an LCAO MO SCF wavefunction obtained from a basis set of Slater-type AO's around the 2 nuclei of the molecule. These are expanded in Legendre polynomials around the centre of mass. The resulting wavefunctions are normalised and used to calculate the static potential.

*Restrictions on the complexity of the program*

The program is limited to an extended basis set of 50 terms, and a maximum shell number of 4.

*Typical running time*

To evaluate a set of MO at 1 value of $r$ takes about $\frac{1}{2}$ sec on the IBM 360/75. Similarly to evaluate a set of static potentials at 1 value of $r$ takes about $\frac{1}{2}$ sec.

*Reference*

[1] A. L. Sinfailam, Computer Phys. Commun. 1 (1970) 445.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 272-287. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTATION OF TOTAL, DIFFERENTIAL AND DOUBLE-DIFFERENTIAL CROSS SECTIONS FOR COMPOUND NUCLEAR REACTIONS OF THE TYPE (a, b), (a, b$\gamma$) AND (a, b$\gamma$-$\gamma$).

## (III) FORTRAN TRANSLATIONS OF THE ALGOL PROGRAMS 'MANDY' AND 'BARBARA'

E. SHELDON, S. MATHUR and D. DONATI

*Nuclear Center, Lowell Technological Institute, Lowell, Massachusetts* 01854, *USA* *

Received 29 April 1971

## PROGRAM SUMMARY (MANDYF)

*Title of program*: (32 characters maximum): MANDYF

*Catalogue number*: ABOJ

*Computer for which the program is designed and others upon which it is operable*

*Computer* Digital PDP-10 (or PDP-9 with 32K core memory)

*Installation*: PDP-10 at Digital Equipment Corp., Maynard, Mass., USA
PDP-9 at Nuclear Center, Lowell Technological Institute, Lowell, Mass., USA

*Operating system or monitor under which the program is executed*: PDP-10 Monitor System or PDP-9 Advanced Software System

*Programming languages used*: FORTRAN-IV

*High speed store required*: 14 K words. *No. of bits in word*: 36

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Disk or Dectape (optional); Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1302

*Reference to other published version of this program*:
*Catalogue number*: ABOA; *Title* : MANDY; *Ref. in CPC*: 1 (1969) 35

*Keywords descriptive of problem and method of solution*: Nuclear, Reaction, Mechanism, Angular Distribution, Statistical, Compound Nucleus, Differential Cross Section, Total Cross Section, Hauser-Feshbach, Satchler, Moldauer, Level-Width Fluctuation, Spin-Parity, Level Assignments, Multipolarity, Multipole Ellipse, Mixing Ratio, Racah Functions, Clebsch-Gordan Coefficient, Racah Coefficient [Wigner 3-*j* and 6-*j* Symbols], Legendre Polynomial, Distribution Function, Transmission Coefficients, Penetrability, *j*-*j* Coupling, Spin-Orbit Coupling, Optical Model, Compound-Elastic Scattering, Inelastic Scattering, Compound Stripping, Transfer.

*Nature of physical problem*

Evaluation of total and differential cross sections in absolute and normalized form for angular distributions in low-energy nuclear reactions of the type (a, a), (a,b), (a,b$\gamma$) or (a,b$\gamma_1$-$\gamma_2$) according to statistical compound-nucleus theory in *j*-*j* coupling formalism. The ALGOL program "MANDY" [1] has been rewritten as "MANDYF" in FORTRAN-IV, retaining the original features of its counterpart.

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* Work supported in part by the National Science Foundation.

*Restrictions on the complexity of the problem*

In the present version of "MANDYF", radiative capture transitions have not been included, and orbital angular momenta in entrance and exit channels have been limited to $l \leqslant 8$, with the number of extra exit channels confined to O3 $\leqslant 40$ for dimensional reasons. To distinguish $0^-$ from $0^+$ nuclear states, appropriate machine-specific procedures have to be devised.

*Reference*

[1] E. Sheldon and R. M. Strang, Computer Phys. Commun. 1 (1969) 35.

## PROGRAM SUMMARY (BARBYF)

*Title of program*: (32 characters maximum): BARBYF

*Catalogue number*: ABOK

*Computer for which the program is designed and others upon which it is operable*

*Computer*: Digital PDP-10 (or PDP-9 with 32 K core memory)

*Installation*: PDP-10 at Digital Equipment Corp., Maynard, Mass., USA
PDP-9 at Nuclear Center, Lowell Technological Institute, Lowell, Mass., USA

*Operating system or monitor under which the program is executed*: PDP-10 Monitor System or PDP-9 Advanced Software System

*Programming languages used*: FORTRAN-IV

*High speed store required*: 16 K words. *No. of bits in a word*: 36

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Disk or Dectape (optional); Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1348

*Reference to other published version of this program*:
*Catalogue number*: ABOB; *Title*: BARBARA; *Ref. in CPC*: 1 (1969) 35.

*Keywords descriptive of problem and method of solution*:
Nuclear, Reaction, Mechanism, Statistical, Compound Nucleus, Angular Correlation, Double-Differential Cross Section, Differential Cross Section, Total Cross Section, Spin-Parity, Level Assignments, Multipolarity, Mixing Ratio, Racah functions, Clebsch-Gordan Coefficients, Racah Coefficients, Fano X-Coefficients [Wigner 3-$j$, 6-$j$ and 9-$j$ Symbols], Legendre Hyperpolynomials, Assocoaited Legendre Functions, Transmission Coefficients, Optical Potential, Penetrability, $j$-$j$ Coupling, Spin-Orbit Coupling, Hauser-Feshbach, Moldauer, Biedenharn-Rose, Satchler, Level-Width Fluctuation, Correlation Function, Inelastic Scattering, Compound Stripping, Transfer.

*Nature of physical problem*

Evaluation of total and double-differential cross sections in absolute and normalized form for angular correlations in low-energy nuclear reactions of the type (a,b$\gamma$) or (a,b$\gamma_1$-$\gamma_2$) according to statistical compound-nucleus theory in $j$-$j$ coupling formalism. The ALGOL program "BARBARA" [1] has been rewritten as "BARBYF" in FORTRAN-IV, retaining the original features of its counterpart.

*Restrictions on the complexity of the problem*

Orbital angular momenta for particles a,b in CN entrance and exit channels are restricted to $l \leq 8$, the number of subsidiary outgoing channels being confined to O3 $\leq$ 40. For discrimination between $0^-$ and $0^+$ nuclear states, appropriate machine-specific procedures have to be devised.

*Typical running time*

About 3-40 minutes per case, depending on the magnitude of the cut-off momenta (normally confined to $l \leq 6$ in practice) and the fineness of the angular variation.

*Reference*

[1] E. Sheldon and R. M. Strang, Computer Phys. Commun. 1 (1969) 35.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 288-297. NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAMS TO AID IN ESTABLISHING GAMMA-RAY DECAY SCHEMES, DCSCH3 AND DCSCH4

B. P. FOSTER *
*Department of Physics, North Texas State University, Denton, Texas* 76203, *USA*
and
D. C. CAMP **
*Lawrence Radiation Laboratory, Livermore, California* 94550, *USA*

Received 7 May 1970
Revised manuscript received 10 February 1971

## PROGRAM SUMMARY (DCSCH3)

*Title of program*: (32 characters maximum) Decay scheme program DCSCH3

*Catalogue number*: ABOF

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360-50. *Installation*: North Texas State University

*Operating system or monitor under which the program is executed*: OS MFT II (HASPII)

*Programming languages used*: FORTRAN IV H

*High speed store required*: 32 806 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer; Disc

*No. of cards in combined program and test deck*: 533

*Keywords descriptive of problem and method of solution*: Nuclear, Atomic, Molecular, Spectra, Energy Level, Gamma Ray, Photon, Quantum, Ritz Combination Principle.

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* Research sponsored in part by a grant from the Faculty Research Fund of North Texas State University.
** Research supported in part by the United States Atomic Energy Commission.

## PROGRAM SUMMARY (DCSCH4)

*Title of program*: (32 characters maximum) Decay scheme program DCSCH4

*Catalogue number*: ABOG

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360-50. *Installation*: North Texas State University

*Operating system or monitor under which the program is executed*: OS MFT II (HASPII)

*Programming languages used*: FORTRAN IV H

*High speed store required*: 32 692 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer; Disc

*No. of cards in combined program and test deck*: 484

*Keywords descriptive of problem and method of solution*: Nuclear, Atomic, Molecular, Spectra, Energy Level, Gamma Ray, Photon, Quantum, Ritz Combination Principle.

*Nature of the physical problem*

The problem of determining a gamma-ray decay scheme and establishing energy levels from the gramma-spectra can be a tedious process. The programs DCSCH3 and DCSCH4 are designed to furnish the experimenter, in a convenient form, the information he needs to carry out this task.

*Method of solution*

The energies of the gamma rays and the energies of the known excited states are fed in as input data. The program then compares, within the specified errors, various comparisons of the sums and differences in the energies of the gamma rays to the excited states and their differences. The programs group and display the results so as to be convenient to the experimenter. In DCSCH3 they are grouped according to the gamma rays involved, while in DCSCH4 they are grouped by excited state.

The programs print out the upper and lower excited states involved in the gamma-ray transitions implied by the comparisons. One of these excited states is a new tentative excited state which was not used in the comparison cited. These tentative states are stored, each with a tag word indicating the gamma ray and the input energy state involved. Later the tentative states are arranged and printed out. The two programs compliment each other so that one has in a convenient format all of the pertinent information to determine the most probable decay scheme.

*Restrictions on the complexity of the problem*

The program as written is restricted to 150 gamma rays and 50 excited states. These restrictions were dictated by the memory of the North Texas State University computer and can be easily increased or decreased.

*Typical running time*

The running times vary with the number of input gamma rays and excited states. An example of typical running times in analyzing the spectrum of $^{76}$Ge [1] running on the IBM 360-50, at North Texas State University, under compiler LEVEL H are shown in table 1 in the conclusion. With the maximum input of 150 gamma-rays and 50 energy states the running time will be between 30 and 45 minutes. Running on the IBM 360-50 with Compiler G, the program takes several times longer. Running similar data on the Livermore CDC 6600 with 107 gammas and 28 excited states it took 15.3 minutes to run using disc storage for 3562 tentative states generated. Recoding to use the CDC 6600 core to store the 3562 tentative excited states generated, the running time was reduced to 3 minutes for the same input data.

*References*

[1] D. C. Camp and B. P. Foster, Nucl. Phys., submitted for publication.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 298. NORTH-HOLLAND PUBLISHING COMPANY

# I. A FORTRAN PROGRAM FOR CALCULATING DEGENERATE RAMAN BANDS OF SYMMETRIC TOPS WITH AN ADAPTATION FOR INFRARED BANDS

F. N. MASRI
*Physics Department, University of Tennessee, Knoxville, Tennessee, USA*
and
I. R. WILLIAMS
*Knoxville College, Knoxville, Tennessee, USA*

Received 24 March 1971

## PROGRAM SUMMARY

*Title of program*: FORTRAN VIBROT I

*Catalogue number*: AAGF

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/91. *Installation*: Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

*Operating system or monitor under which the program is executed*: OS 360

*Programming language used*: FORTRAN IV

*High speed store required*: 14 500 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Printer

*No. of cards in combined program and test deck*: 265

*Reference to other published version of this program*: *Catalogue number*: AAGC; *Title*: VIBROT I; *Ref. in CPC*: 1 (1970) 349.

*Keywords descriptive of problem and method of solution*: Molecule, Raman, Scattering, Spectra, Symmetric Tops, Coriolis Coupling.

*Nature of the physical problem*
This program solves the same physical problem as program VIBROT I. The original program has been translated into FORTRAN IV from ALGOL. The logic, the test data and the output format are all virtually identical. The total CPU time is 11 seconds.

## ADAPTATION SUMMARY

*Title of adaptation*: FORTRAN VIBROT I FOR INFRARED

*Adaptation number*: 0001

*Reference to original program*: *Catalogue number*: AAGF; *Title*: FORTRAN VIBROT I; *Ref. in CPC*: this issue

*Authors of original program*: F. N. Masri and I. R. Williams

*No. of cards required to effect adaptation (including directive cards)*: 27

*Additional Keywords*: Infrared, Absorption.

*Nature of the adaptation*
A direct interchange of a section of the inner block of the program allows the calculation of infrared bands in place of Raman bands.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 299. NORTH-HOLLAND PUBLISHING COMPANY

# II. A FORTRAN PROGRAM FOR CALCULATING DEGENERATE RAMAN BANDS OF SPHERICAL TOPS WITH AN ADAPTATION FOR INFRARED BANDS

F. N. MASRI
*Physics Department, University of Tennessee, Knoxville, Tennessee, USA*
and
I. R. WILLIAMS
*Knoxville College, Knoxville, Tennessee, USA*

Received 24 March 1971

## PROGRAM SUMMARY

*Title of program*: FORTRAN VIBROT II

*Catalogue number*: AAGG

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 1130. *Installation*: Knoxville College, Knoxville, Tennessee, USA

*Operating system or monitor under which the program is executed*: OS 1130

*Programming languages used*: FORTRAN IV

*High speed store required*: 4000 words. *No. of bits in a word*: 16

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Printer

*No. of cards in combined program and test deck*: 229

*Reference to other published version of this program*: *Catalogue number*: AAGE; *Title*: VIBROT II; *Ref. in CPC*: 2 (1971) 87.

*Keywords descriptive of problem and method of solution*: Molecule, Raman, Scattering, Spectra, Spherical Tops, Coriolis Coupling.

*Nature of the physical problem*

This program solves the same physical problem as program VIBROT II. The original program has been translated into FORTRAN IV from ALGOL. The logic, the test data and the output format are all virtually the same.

## ADAPTATION SUMMARY

*Title of adaptation*: FORTRAN VIBROT II FOR INFRARED

*Adaptation number*: 0001

*Reference to original program*: *Catalogue number*: AAGG; *Title*: FORTRAN VIBROT II; *Ref. in CPC*: this issue.

*Authors of original program*: F. N. Masri and I. R. Williams

*No. of cards required to effect adaptation* (including directive cards): 27

*Additional Keywords*: Infrared, Absorption.

*Nature of the adaptation*

A direct interchange of a section of the inner block of the program allows the calculation of infrared bands in place of Raman bands.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 301-321. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTER SIMULATION OF EXTENDED DEFECTS IN METALS*

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J. R. BEELER Jr.
*Department of Materials Engineering, North Carolina State University, Raleigh, North Carolina, USA*

and

R. D. BOURQUIN
*Battelle-Northwest, Richland, Washington, USA*

Received 28 September 1970
Revised manuscript received 14 May 1971

## PROGRAM SUMMARY

*Title of program* : GRAINS

*Catalogue number*: ACQY

*Computer for which the program is designed and others upon which it is operable*

*Computer*: UNIVAC 1108. *Installation*: Computer Sciences Corporation, Richland, Washington, USA

*Programming languages used*: FORTRAN

*High speed store required*: 47,944 words. *No. of bits in a word*: 36

*Is the program overlaid*? No

*No. of magnetic tapes required*: 0–4, depending upon input and output options

*What other peripherals are used*: Card Reader; Line Printer; CAL-COMP Plotter (requires machine language control routines)

*No. of cards in combined program and test deck*: 1817

*Keywords descriptive of problem and method of soluton*: Solid State, Discrete Lattice Theory, Computer Simulation, Grain Boundaries, Quasi-dynamic and Fully Dynamic Methods of Solution, Classical Mechanics, Interatomic Potential Functions.

*Nature of physical problem*

The program is designed to determine the atomistic structure of extended defects in crystals with cubic structure, and their interactions with point defects. The extended defects which can be studied are grain boundaries, twin boundaries, free surfaces, cracks and dislocations. In addition, elementary aspects of grain boundary sliding can be studied.

*Method of solution*

The lowest potential energy configuration for a given extended defect is computed using the quasi-dynamical method of Gibson et al. [1]. This method develops a many-body description of the equilibrium configuration on the basis of newtonian mechanics. The central difference approximation is used to numerically integrate the equations of motion for every atom in the crystallite simultaneously. The interatomic forces used in solving the equations of motion are obtained from a short-range, semi-empirical atomic interaction function.

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* This paper is based on work performed by Battelle-Northwest under U. S. Atomic Energy Commission Contract AT(45-1)-1830 [Dahl and Bourquin]; by the Hanford Engineering Development Laboratory, Richland, Washington, operated by WADCO Corporation, a subsidiary of Westinghouse Electric Corporation, under U. S. Atomic Energy Commission Contract AT(45-1)-2170 [Dahl]; and by the North Carolina State University under U. S. Atomic Energy Commission Contract AT(40-1)-3912 and Air Force Material Laboratory Contract F33615-68-C-1012 [Beeler].

*Restrictions on the size of the extended defect*

The capability of the program for studying defect interactions as a function of relative positions is limited by the size of the computational cell. This, in turn, is limited by the computer storage capacity. The largest number of atoms which can be considered in a crystallite is 3500. About half of these are contained in an enveloping mantle of immovable atoms which induces the proper crystal structure and volume cohesive forces. The remainder can be moved arbitrarily and comprise the central portion of the crystallite. This set of movable atoms is called the computational cell.

*Typical running time*

The time required on 1108 UNIVAC computer for the construction of a grain boundary and convergence to a structure in which the total internal energy of the system did not vary by more than 0.001 eV was about 10 minutes for a cell containing approximately 2 000 atoms. The time for solution is dependent upon the convergence criterion, and is approximately linearly dependent upon the number of movable atoms.

*Unusual features of the program*

A variety of orientations for the defected crystallite are available. Either the axis (linear defect) or the habit plane normal (planar defect) for the extended defect under consideration can be oriented along any one of the directions ⟨100⟩, ⟨100⟩,⟨111⟩ and ⟨112⟩. The dynamical stability of an equilibrium configuration obtained via the quasi-dynamical method, effectively at absolute zero temperature, can be tested at an arbitrary non-zero temperature by assigning a randomly directed velocity vector to each atom in the computational cell. These randomly directed velocity vectors have a common magnitude determined by the test temperature.

*Reference*

[1] J. B. Gibson, A. N. Goland, M. Milgram and G. H. Vineyard, Phys. Rev. 120 (1960) 1229.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 322-330. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTER ANALYSIS OF MÖSSBAUER SPECTRA*

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Received 30 March 1971

## PROGRAM SUMMARY

*Title of program*: MÖSSBAUER FITTING PROGRAM

*Catalogue number*: ABIB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360-75; IBM 360-50. *Installation*: University of Illinois; Kansas State University

*Operating system or monitor under which the program is executed*

*Programming languages used*: FORTRAN IV

*High speed store required*: 32K words. *No. of bits in a word* : 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer; Card Punch

*No. of cards in combined program and test deck*: 1078

*Keywords descriptive of problem and method of solution*: Nuclear, Solid State, Mössbauer Effect, Least-Squares Fitting, Lorentzian Line Shape.

*Nature of physical problem*

Experimental Mössbauer data are fitted to a sum of lorentzian lines. The program allows for several types of background: flat, sloping or parabolic. The parameters for the background are fitted simultaneously with the lorentzian parameters.

*Method of solution*

The least-squares fit is performed using a Gauss-Newton iteration procedure. Each lorentzian line is characterized by three parameters: intensity (given in counts), half width at half maximum (given in channel numbers) and a line position (given in channel number). The width and intensity parameters may be restricted to be multiples of one another. However, the line positions cannot be so restricted.

*Restrictions to the complexity of the program*

At present the program is dimensioned such that the maximum number of parameters allowed is 50 and the maximum number of data points is 512. Either of these restrictions may be removed by increasing the appropriate dimensioned variables.

*Typical running time*

The execution time is of course dependent on the number of parameters and the number of data points as well as on the initial estimates of all the parameters. Using the IBM 360-50 at Kansas State University with a G level compiler twelve lorentzian lines with a flat background (37 parameters) were fitted to 256 data points in approximately 5 minutes. Using the H level compliler this is reduced to 2.5 minutes. Using a Model 360-75 the execution time is less than 20 seconds.

*Unusual features of the program*

By suitably choosing certain restrictions on the parameters a variety of physical models can be imposed on the data and the goodness of fit checked. By assigning certain values to control parameters the informational output of the program can be controlled in a convenient manner.

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* Work supported in part by National Science Foundation Grant No. GP-26282.

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‡ Present address: Department of Physics, Kansas State University, Manhattan, Kansas 66502, USA.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 331-340. NORTH-HOLLAND PUBLISHING COMPANY

# ELECTROMAGNETIC M1 REDUCED TRANSITION PROBABILITIES FOR PURE AND MIXED NILSSON STATES IN ODD *A* NUCLEI‡

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Received 2 April 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): MIXING

*Catalogue number*: ABQB

*Computer for which the program is designed and others upon which it is operable*:

*Computer*: Burroughs B3500. *Installation*: Burroughs Co., Argentina, Buenos Aires

*Operating system or monitor under which the program is executed*: Burroughs MCP

*Programming languages used*: FORTRAN IV

*High speed store required*: 5000 words. *No. of bits in a word*: 48

*Is the program overlaid*? No

*No. of magnetic tapes required* None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 646

*Keywords descriptive of problem and method of solution*: Nuclear, Reduced Transition Probability, Orbitals, Admixtures, Matrix Elements, Nilsson Coefficients, Clebsch-Gordan Coefficients, Wavefunctions.

*Nature of the physical problem*

Program MIXING computes M1 reduced transition probabilities between pure Nilsson single particle states and also between states mixed by Coriolis and/or $\Delta N = 2$ interactions.

*Method of solution*

M1 reduced transition probabilities are calculated using the formulae given by Nilsson [1]. The computation of the transition matrix elements is performed by the subroutine GM1. When the states are not pure, the program computes the transition probability taking into account the admixtures in the wavefunction. The resulting value given in units of ($e^2 \times cm^2$) is printed.

*Restrictions on the complexity of the problem*

Mixed states with two or more components having the same values of the quantum numbers $N$ and $\Omega$ are not allowed.
Allowable maximum spin is 21/2. For higher values further factorials must be added to the data in the function CLEBSH.
The program permits up to 20 admixtures in the wavefunction of each state and 8 Nilsson coefficients $a_{l\Lambda}$ for each orbital.

*Unusual features of the program*

An option is provided to normalize the input Nilsson coefficients when necessary. This is performed by the subroutine NORMAL. The quantum numbers $l$ and $\Lambda$ corresponding to each coefficient are calculated and printed.

*Reference*

[1] S. G. Nilsson, Kgl. Danske Videnskab. Selskab Mat. Fys. Medd. 29 (1955) no. 16.

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‡ Work done under the partial auspices of the Consejo Nacional de Investigaciones Científicas y Técnicas, Buenos Aires, Argentina.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 341-352. NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAM FOR CALCULATING LEED INTENSITIES USING BAND STRUCTURE-MATCHING FORMALISM

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Received 13 May 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): LEED

*Catalogue number*: ACMH

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/67. *Installation*: IMAG, CEDEX 53, Grenoble

*Operating system or monitor under which the program is executed*: OS 360/67 WATFOR compiler

*Programming languages used*: FORTRAN IV

*High speed store required*: 7214 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1087

*Keywords descriptive of problem and method of solution*: Solid State, LEED, Low Energy Electron Diffraction, Band Structure, Crystal, Surface, Schrödinger Equation, Reciprocal Lattice Vectors.

*Nature of physical problem*

The program computes Low Energy Electron Diffraction (LEED) intensities using the band structure-matching formalism [1-3]. It calculates the intensity as a function of incident energy or angle for the (001) surface of cubic lattices (sc, fcc or bcc) as well as calculating band structures.

*Method of solution*

The LEED intensities are obtained by matching at the surface the solutions of Schrödinger's equation inside and outside the crystal.

*Restrictions on the complexity of the problem*

The crystals are semi-infinite with a step surface potential barrier. The program is designed for calculating LEED intensities from the (001) face only.

*Typical running time*

The time depends crucially on the energy and the number of reciprocal lattice vectors but for most applications it is between 5 and 30 seconds per point.

*References*

[1] D. S. Boudreaux and V. Heine, Surface Sci. 8 (1967) 426.
[2] V. Hoffstein and D. S. Boudreaux, Phys. Rev. Letters 25 (1970) 512.
[3] V. Hoffstein and D. S. Boudreaux, Phys. Rev. B15 (1971) 2447.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 353-359. NORTH-HOLLAND PUBLISHING COMPANY

# BOUND STATE SOLUTION OF THE TWO-NUCLEON SCHRÖDINGER EQUATION WITH TENSOR FORCES

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*and Istituto Nazionale di Fisica Nucleare, Sezione di Pisa, Pisa, Italy*

Received 17 May 1971

## PROGRAM SUMMARY

*Title of program*: DEUT

*Catalogue number*: ABGE

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 7090. *Installation*: Pisa University, Pisa, Italy

*Operating system or monitor under which the program is executed*: IBSYS Version 13 (IBJOB Processor Version 5)

*Programming languages used*: FORTRAN IV

*High speed store required*: 23 000 words. *No. of bits in a word*: 36

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? None

*No. of cards in combined program and test deck*: 968

*Keywords descriptive of problem and method of solution*: Nuclear, Two-Nucleon, Neutron-Proton, Schrödinger Equation, Deuteron, Tensor Forces, Wavefunctions, Electric Quadrupole Moment, D-Wave Percentage.

*Nature of physical problem*

Subroutine DEUT is a FORTRAN IV subroutine designed to calculate the binding energy and wavefunction of the neutron-proton $J = 1^+$ bound state when the interaction between the particles is described by a given combination of central, tensor and spin-orbit potentials with or without a hard core. This subroutine may also be employed in nuclear Hartree-Fock calculations using an effective nucleon-nucleon potential containing a tensor component, and in all those eigenvalue problems reducible to that of a particle moving under the influence of a force containing a tensor component.

*Method of solution*

The method of calculation employed follows very closely the treatment presented in ref. [1]. The requirements that the wavefunctions vanish at the origin and at infinity cause this to be an eigenvalue problem: the technique used for the solution involves a direct numerical integration of the differential equations with middle point matching, accompanied by the iterative application of a suitable correction formula for a trial value of the binding energy.

*Restrictions on the complexity of the problem*

The interparticle potentials considered in the program are the Hamada-Johnston potential [2] and the Reid hard-core or soft-core potentials [3]. To use subroutine DEUT in the case of some other potential one must simply re-write the subprogram POT.

*Typical running time*

The test case requires 85 seconds to compile and 15 seconds to run on the IBM 7090 computer at Pisa University.

*References*

[1] L. Lovitch and S. Rosati, Phys. Rev. 140 (1965) B877.
[2] T. Hamada and I. D. Johnston, Nucl. Phys. 34 (1962) 382.
[3] R. V. Reid, Ann. Phys. 50 (1968) 411.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 360-367. NORTH-HOLLAND PUBLISHING COMPANY

# AMPLITUDES FOR SCATTERING OF ELECTRONS BY HYDROGENIC AND ALKALI-LIKE ATOMIC SYSTEMS

D. L. MOORES

*Physics Department, University College, London W.C.1., UK*

Received 24 June 1971

## PROGRAM SUMMARY

*Title of program*: SCATTERING AMPLITUDES

*Catalogue number*: AAGH

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/65. *Installation*: UCL London

*Operating system*: OS/360

*Programming language used*: FORTRAN IV

*High speed store required*: 6952 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? None

*No. of cards*: 675

*Keywords*: Atomic, Scattering, Reactance Matrix, Elastic, Inelastic, Scattering Amplitudes, Electron, Hydrogenic, Alkali-like, Cross Section.

*Nature of physical problem*

Amplitudes for elastic and inelastic scattering of electrons by hydrogenic and alkali-like atomic systems are computed from reactance matrix elements, assumed to be punched on cards in a standard format.

*Method of solution*

Data are sorted and checked and the summations required are performed.

*Restrictions on complexity of the problem*

Transitions from the ground state to up to 3 final s- and up to 2 p-states can be handled. Coupling to atomic states with $l < 3$ only is considered. Otherwise, dimensions may be altered to increase the scope of the program.

*Typical running time*

Compile time 15 sec, execution of sample data 3 sec.

*Unusual features*

Double length, 8 bytes per word is used for all non-integer variables.

COMPUTER PHYSICS COMMUNICATIONS 3 (1971) 368-380. NORTH-HOLLAND PUBLISHING COMPANY

# ANALYSIS OF A VARIABLE SPECTRCSCCPIC DOUBLE STAR

D. HERBISON-EVANS and N. R. LOMB
*School of Physics, Sydney University N.S.W.2006, Australia*

Received 23 June 1971

## PROGRAM SUMMARY

*Title of program*: BISPEC

*Catalogue number*: AACE

*Computer for which the program is designed and others upon which it is operable*

*Computer*: English Electric KDF9. *Installation*: Basser Computing Dept. Sydney Universtiy

*Operating system or monitor under which the program is executed*: KIDSGROVE COMPILER

*Programming languages used*: ALGOL

*High speed store required*: 20K. *No. of bits in a word*: 48

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Paper Tape Reader; Line Printer

*No. of lines in combined program and test deck*: Approximately 550

*Keywords descriptive of the problem and method of solution*: Astrophysics, Doppler Shift, Variable-star, Spectroscopic-binary-star, Minimisation, Simplex Method.

*Nature of the physical problem*

Measurements of the Doppler shifts of the spectral lines of a double star at different times can be used to derive the velocities of the stars at these times. The program 'bispec' derives the orbital parameters (mean velocities, amplitudes, longitude of periastron, epoch of periastron, eccentricity, orbital period, and period of rotation of the line of apsides) of the stars from these velocities. The program will also find the best fitting sine wave (amplitude, period and epoch of zero phase) to the velocities, measured at various times, of an oscillating star. It can solve both problems simultaneously if one of the members of a double star is oscillating. This has been done for the star $\alpha$ Virginis [1].

*Method of solution*

A test set of orbital and oscillation parameters is used to produce calculated values of the velocities at the times of observation. A total residual is produced by summing the weighted squares of the differences between corresponding calculated and observed velocities. A simplex method [2] is used to search the parameters so as to minimise this residual.

*Restrictions*

The program can cope with a maximum of 605 sets of observations, although this is easily altered, and only one of the stars can be oscillatory. The program uses the third order Newton-Raphson solution of Kepler's equation.

*Typical running time*

The time taken for a complete minimisation depends on the proximity of the initial parameters to the best fitting parameters, and the dimensionality of the search.

*Unusual features*

The program allows any subset of the parameters to be searched for a minimum residual. It enters a machine code loop for greater speed if the line of apsides is assumed fixed and neither of the stars is oscillatory. It can be used to print out the residuals on a grid of values of any 2 parameters. The program produces the standard deviations of the final parameters. It will also print out an analysis of the stars' motions at the epochs of observation, if required.

*References*

[1] N. R. Lomb, R. R. Shobbrook and D. Herbison-Evans, Monthly Notices Roy. Astron. Soc., to be published.
[2] J. A. Nelder and R. Mead, Computer J. 7 (1965) 308.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 394-419. NORTH-HOLLAND PUBLISHING COMPANY

# A TRACK MATCHING PROGRAM FOR BUBBLE CHAMBER PHOTOGRAPHS*

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*Massachusetts Institute of Technology, Laboratory for Nuclear Science, Cambridge, Mass., USA*

and

V. PLESS

*Air Force Cambridge Research Laboratories, Cambridge, Mass., USA*

Received 15 March 1971

## PROGRAM SUMMARY

*Title of program*:(32 *characters maximum*): MATCH

*Catalogue number*: ABCB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360-65. *Installation*: Massachusetts Institute of Technology Laboratory for Nuclear Science

*Operating system or monitor under which the program is executed*:OS/360

*Programming Languages used*:FORTRAN

*High speed store required*:$\approx$ 30 K *words*. *No. of bits in a word*: 32

*Is the program overlaid*? Yes (for the test run)

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 3338

*Keywords descriptive of problem and method of solution*: Nuclear, High Energy, Bubble Chamber, Track Matching, First Order Optics.

*Nature of physical problem*

Bubble chamber events are photographed by three cameras. Given sets of unlabeled track measurements in each of the three views, the program labels corresponding tracks.

*Method of solution*

There are two distinct steps in the solution:

(i) We use the simplest possible geometric situation (all indices of refraction set to 1) to find potential triples of tracks.

(a) We eliminate all pairs of tracks which could not possibly have come from the same track in space. A pair is defined as a track measurement in view $i$ together with a track measurement in view $j$ ($i \neq j$).

(b) We construct for all triples of tracks surviving the pair test an estimator which in principle should be zero if the three tracks belong to the same track in space. Because of our crude geometrical approximation the estimator cut-off must be set high and some related triples will in general remain after the test.

(ii) We now rely on logic to separate related triples. A set of related triples can be shown to form an equivalence class. The equivalence classes are processed through a routine which finds the *maximal* independent set of triples for the class.

*Restrictions on the complexity of the program*

The program is quite general since it can handle an unequal number of tracks in each view. For example the input could consist of the track measurements for an interaction plus random extraneous tracks in each view. Furthermore, since tracks measured with automatic devices usually have large gaps or sometimes sections missing entirely, the minimum percentage overlap between the tracks of a pair is an adjustable parameter.

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* This work has been supported in part through funds provided by the U.S. Atomic Energy Commission under Contract No. AT(30-1) 2098.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 420-426. NORTH-HOLLAND PUBLISHING COMPANY

# SU3 FRACTIONAL PARENTAGE IN THE 1p-SHELL

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*Institut de Physique Nucléaire, 43 Boulevard du 11 novembre 1918, 69 Villeurbanne, France*

Received 23 November 1970
Revised manuscript received 6 July 1971

## PROGRAM SUMMARY

*Title of program* (32 characters maximum): 1PSHELL SU3 FRACTIONAL PARENTAGE

*Catalogue number* : ABOL

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: S.I.A. International, Agence de Lyon (France)

*Operating system or monitor under which the program is executed*: CDC Scope 3.2

*Programming languages used*: FORTRAN

*High speed store required*: 19 905 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer for Driver

*No. of cards in combined program and test deck*: 1468

*Keywords descriptive of problem and method of solution*: Nuclear, Atomic, Nuclear Spectra, Nuclear Structure, Atomic Spectra, Atomic Structure, SU3, Fractional Parentage Coefficient.

*Nature of the physical problem*

Using Elliott's SU3 model we calculate the fractional parentage coefficients (F.P.C.) occurring in matrix elements for various $m$-particles operators ($m = 1, 2, 3, 4$) and in reduced widths of the p-shell nuclei for deuterons, tritons and $\alpha$-particles.

*Method of solution*

The $\langle p^n\{|p^{n-1}p\rangle$ F.P.C. given by Jahn and van Wieringen [1] are tabulated and the

$\langle p^n\{|p^{n-2}p^2\rangle, \langle p^n\{|p^{n-3}p^3\rangle$ and $\langle p^n\{|p^{n-4}p^4\rangle$

coefficients are calculated using the Smirnov and Chlebowska expressions [2]. We use a modified version of Tamura's subroutines [3,4] for the geometrical coefficients which appear in these formulas.

*Unusual features of the program*

Before the calculation, the core of the computer must be cleared (control card LOC(100,107 700).

*Typical running time*

The average calculation times are: less than 1 msec for the $n|n-1$ coefficients, about 30 msec for the $n|n-2$, between 200 and 700 msec for the $n|n-3$ and about 2 sec for the $n|n-4$ ones. The test run (including compilation) requires 26 sec on the CDC 6600 computer.

*References*

[1] H. A. Jahn and H. van Wieringen, Proc. Roy. Soc. A209 (1951) 502.
[2] Yu. F. Smirnov and D. Chlebowska, Nucl. Phys. 26 (1961) 306.
[3] T. Tamura, Oak Ridge National Laboratory, Report ORNL-3877 (1965).
[4] T. Tamura, Computer Phys. Commun. 1 (1970) 337.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 427-432. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM TO CALCULATE INTERNAL CONVERSION COEFFICIENTS FOR ALL ATOMIC SHELLS WITHOUT SCREENING

O. DRAGOUN* and G. HEUSER
*Max-Planck-Institut für Kernphysik, Heidelberg, Germany*

Received 30 July 1971

## PROGRAM SUMMARY

*Title of program*: INTERNAL CONVERSION COEFFICIENTS

*Catalogue number*: ABGF

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 3300. *Installation*: Max-Planck-Institut für Kernphysik, Heidelberg, Germany

*Operating system or monitor under which the program is executed*: MSOS

*Programming languages used*: FORTRAN IV

*High speed store required*: 4659 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*: Card Reader; Line Printer

*No. of cards in the combined program and test deck*: 773

*Keywords descriptive of the problem and method of solution*: Nuclear, Atomic, Internal, Conversion, Coefficient, Coulomb, Screening, Gamma Function, Hypergeometric Series, Hypergeometric function.

*Nature of the physical problem*

The program calculates internal conversion coefficients for all atomic subshells from K up to $Q_1$. The formulas used [1] are based on an analytical solution of the Dirac equation for electrons in the pure Coulomb field of a point nucleus. The finite-nuclear-size correction is included. The conversion coefficients computed with this program and corrected approximately for atomic screening [2] were found to be in good agreement with experiment. The method is especially useful in cases in which no precise conversion coefficients are available (outer atomic shells, low atomic numbers, high transition energies).

*Method of solution*

The gamma function of complex argument is evaluated using the asymptotic and recurrence formulas. The hypergeometric function of complex variables, ${}_2F_1(a,b;\ c;\ z)$, is computed from the hypergeometric series inside the circle of convergence and by an analytical continuation outside this region.

*Restrictions on the complexity of the program*

The program was tested successfully for all atomic subshells ($K \ldots Q_1$), atomic numbers $Z \leq 100$, for electric and magnetic multipoles with $1 \leq L \leq 5$ and for transition energies higher than the electron binding energy in the pure Coulomb field up to 17 MeV.

*Typical running time*

The evaluation of the K-shell conversion coefficient takes about two to six seconds on the CDC 3300. To calculate the $P_5$ subshell conversion coefficient for the $2^5$ pole electric transition requires about 70 seconds.

*References*

[1] R. F. O'Connell and C. O. Carroll, in: Internal conversion processes, ed. J. H. Hamilton (Academic Press, New York, 1966) p. 333.
[2] O. Dragoun, P. Jahn, H. Allers, M. Vobecký and H. Daniel, Phys. Letters 28B (1968) 251.

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* Now at the Nuclear Research Institute, Řež near Prague, Czechoslovakia.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 433-442. NORTH-HOLLAND PUBLISHING COMPANY

# ENERGY-LOSS STRAGGLING OF HEAVY CHARGED PARTICLES*

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*and Max-Planck-Institut für Kernphysik, Heidelberg, Germany*
*and University of Oregon, Eugene, Oregon* 97403, *USA* †

and

Nelson JARMIE
*Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico* 87544, *USA*

Received 29 July 1971

## PROGRAM SUMMARY

*Title of program*: STRAGL

*Catalogue number*: ABON

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: Los Alamos

*Operating system or monitor under which the program is executed*: SCOPE 3.0

*Programming lanuages used*: FORTRAN IV

*High speed store required*: 44500 *words*. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1307

*Keywords*: Nuclear, Atomic, Energy Straggling. Energy Loss, Particle Beams, Vavilov Distribution, Distant Collision Correction, Thin Absorbers, Landau Distribution.

*Nature of the physical problem*

STRAGL calculates the energy-loss distribution (straggling) of a monoenergetic beam of charged particles, heavier than electrons, after it has passed through a thin absorber.

*Method of solution*

The energy-loss distribution is calculated using the formulas of Vavilov [1] with the modification due to Shulek et al. [2] which includes the effects of bound electrons. The calculation extends and corrects the older regions of the Landau distribution and the gaussian straggling distribution. The mean ionization potential of the absorber can either be supplied or will be calculated by the program. The output listing provides various parameters of interest used in the calculation, the mean energy loss, most probable energy loss, and the fwhm of the energy distribution. The distribution is then plotted on the listing directly, and a table is printed that lists the values of the distribution directly in probability per unit energy versus the energy loss.

*Restrictions on the complexity of the problem*

The beam is assumed to be monoenergetic and heavier than electrons. There is no high energy limit. The low energy and the large thickness limits are determined by the restriction that the mean energy loss should not be more than 10 to 20% of the initial particle energy. For *very* thin absorbers (for example, a few keV energy loss), the calculation also fails: for details see the main text.

*References*

[1] P. V. Vavilov, Soviet Phys. JETP 5 (1957) 749.
[2] P. Shulek, B. M. Golovin, L. A. Kulyukina, S. V. Medved' and P. Pavlovich, Soviet J. Nucl. Phys. 4 (1967) 400.

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* Work performed under the auspices of the U. S. Atomic Energy Commission.

† Present address.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 443-448. NORTH-HOLLAND PUBLISHING COMPANY

# KINEMATICAL PARAMETERS OF NUCLEAR REACTIONS*

Amy WOLFRAM, C. Fred MOORE and W. Rory COKER
*Center for Nuclear Studies, University of Texas, Austin, Texas 78712, USA*

Received 16 July 1971

## PROGRAM SUMMARY

*Title of program*: NUCLEAR SPECTRA

*Catalogue number*: ABOM

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: The University of Texas Computer Center

*Operating system or monitor under which the program is executed*: UT-2

*Programming languages used*: FORTRAN

*High speed store required*: 77 777 *words*. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: One

*What other peripherals are used*? Card Reader; Line Printer for Driver

*No. of cards in combined program and test deck*: 598

*CPC Library data deck used*

*Catalogue number*: AAA*; *Title*: DATA FOR ABOM

*No. of cards in data deck*: 12980

*Keywords descriptive of problem and method of solution*: Nuclear, Reactions, Reaction Kinematics Energy Spectrum, Reaction Products, Q-Value, Nuclear Masses, Mass Excess, Excitation Energy, Level Scheme, Level Spin, Level Parity.

*Nature of the physical problem*

The program calculates various parameters of nuclear reactions: given the charge and mass of the projectile, target, and emitted nuclei of interest, the incident energy and the laboratory angle at which reaction products are observed, the program calculates the energy, inverse velocity, and momentum of the final reaction products as well as the $Q$-value of the reaction at the given reaction angle. The program also outputs the specific residual nuclear states excited.

*Method of solution*

The program does a classical relativistic calculation to obtain the kinetic energy of the emitted nucleus and the $Q$-value of a specified nuclear reaction. The calculations are based on first principles of conservation of energy and momentum and are accurate to the number of significant bits in the computer word length. A complete library of data on nuclear levels is available to and used by the program.

*Restrictions on the complexity of the problem*

Execution is faster if targets are considered in order of ascending mass number, $A$. The code can accomodate only four hundred individual reactions per data set unless the fields in which the relevant parameters are stored are enlarged.

*Typical running time*

The running time for a calculation involving one projectile incident at one energy on four targets with five nuclei emitted at one angle is 14 seconds.

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* Work supported in part by the Robert A. Welch Foundation and the U. S. Atomic Energy Commission.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 449-454. NORTH-HOLLAND PUBLISHING COMPANY

# GAMMA-RADIATION DOSIMETRY FOR ARBITRARY SOURCE AND TARGET GEOMETRY*

Lincoln B. HUBBARD
*Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA*
*and Furman University, Greenville, South Carolina, USA*

Received 3 March 1971

## PROGRAM SUMMARY

*Title of program*: DOSE1

*Catalogue number*: ACMG

*Computer for which the program is designed and others upon which it is operable.*

*Computer*: IBM 360/75 and 91. *Installation*: Oak Ridge National Laboratory

*Operating system or monitor under which the program is executed*: OS360

*Programming languages used*: FORTRAN IV(H)

*High speed store required*: 25 500 *words*. *No. of bits in word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals used*: Card Reader and Printer

*No. of cards in combined program and test deck*: 351

*Keywords descriptive of problem and method of solution*: Radiation, Dosimetry, Dose, Absorption, Gamma-ray, Photon, Energy Deposition.

*Nature of the physical problem*

The program DOSE1 calculates the first collision dose in the formalism of absorbed fractions [1] for gamma-rays in arbitrary finite geometry of source, absorber and target. The basic unit of the program is the subroutine ATINTG which calculates the attenuation term

$$\exp[-\int_{r_1}^{r_2} \mu(r)\,\mathrm{d}r] ,$$

where the line integral is taken along the straight line path from $r_1$ to $r_2$. This attenuation term is applicable to all examples of exponential absorption in an arbitrary absorption distribution, provided that, the linear absorption coefficient, $\mu$, is known as a function of position.

*Method of solution*

The total volume, including both source and target, is subdivided into small parallelepipeds. The source strength and target absorption for each of these elementary volumes are placed at the geometric center. The absorption is calculated as exponential, $\exp(-\mu x)$, for each elementary volume traversed from the center of the source volume to the center of target volume. The contributions for all sources are summed to give point-specific absorbed fractions for each elementary volume. The total absorbed fraction is the average of the point functions. The approach used here differs markedly from the current dosimetry procedure of using the Monte-Carlo method [2].

*Restrictions on the complexity of the problem*

This method is exact in principle for only the first collision dose, since exponential absorption is used.

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* Research sponsored in part by the U.S. Atomic Energy Commission under contract with Union Carbide Corporation and in part by a grant to Furman University by the College Science Improvement Programs of the National Science Foundation.

For bodies whose linear dimensions are much less than the mean free photon path, this is a reasonable approximation. For slightly larger volumes an approximation assuming an effective absorption coefficient [3] has some validity.

The program is completely general in terms of geometry. It is suitable for distributed or point sources, both internal and external to the target. For some situations the dimensions of the subscripted variables would require modification.

*Typical running time*

The execution time for this program is very sensitive to the input parameters. Execution time will vary approximately as $N^{7/3}$ where $N$ is the number of elementary sub-volumes. For the rather simple problem exhibited in the sample output the execution times are 0.6 seconds on the IBM-360/75 and 0.2 seconds on the IBM-360/91. Compile times are 11 seconds and $2\frac{1}{2}$ seconds for the IBM-360/75 and IBM-360/91, respectively.

*References*

[1] R. Loevinger and M. Berman, Phys. Med. Biol. 13 (1968) 205.

[2] W. H. Ellet, G. L. Brownell and A. R. Reddy, Phys. Med. Biol. 13 (1968) 219.

[3] R. Loevinger, J. G. Holt and G. J. Hine, in: Radiation dosimetry, eds. G. J. Hine and G. L. Brownell (Academic Press, New York, 1956) ch. 17.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 455-469. NORTH-HOLLAND PUBLISHING COMPANY

# CALCULATION OF ELECTRIC QUADRUPOLE RADIAL MATRIX ELEMENTS FOR COULOMB EXCITATION

M. SAMUEL and U. SMILANSKY

*Department of Nuclear Physics, Weizmann Institute of Science, Rehovot, Israel*

Received 2 April 1971

## PROGRAM SUMMARY

*Title of program*: ITER

*Catalogue number*: ABQC

*Computer for which the program is designed and others upon which it is operable*:

*Computer*: GOLEM *Installation*: Weizmann Institute, Rehovot,
CDC 3400 Tel-Aviv University

*Operating system or monitor under which the program is executed*: Disk 1. Operable also under Diskard (GOLEM computer)

*Programming language used*: FORTRAN IV

*High speed store required*: 7700 words (in GOLEM computer)

*No. of bits in a word*: 75 in GOLEM computer: 48 in CDC 3400

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*: Card Reader; Line Printer

*No. of cards in combined program and test deck*: 484

*Keywords descriptive of problem and method of solution*: Nuclear, Coulomb Excitation, Inelastic Scattering, Coulomb Barrier, Recursion

*Nature of physical problem*

Radial matrix elements $M^{-3}_{l_i l_f}$ for E2 or M1 Coulomb excitation [1] are calculated up to $l_i = 500$ with $l_f = l_i$, $l_i \pm 2$. These elements are used in the calculation of scattering amplitudes associated with inelastic scattering of charged particles from nuclei, by partial waves expansion. When non-Coulomb short range forces are included, these elements apply to large $l$-values [2]. Coulomb interaction is important even at energies high above the Coulomb barrier, and a few hundred partial waves have to be included [3].

*Method of solution*

Monopole matrix elements $M^{-1}_{l\,l}$ are calculated by a downward recursion, starting at $l =$ LAAX. They are normalized by a direct calculation of $M^{-1}_{1\,1}$ Quadrupole matrix elements with $l_f = l_i + 2$ are calculated also by a downward recursion starting at $l =$ LMAX. Upward recursions are used to calculate $M^{-3}_{l\,l}$ and $M^{-3}_{l+2\,l}$. These recursions start from directly calculated elements with low $l$-values and use the elements $M^{-3}_{l\,l+2}$. The formulae used are based on refs. [1] and [4]. LMAX and LAAX are chosen to give $10^{-7}$ accuracy in all quadrupole matrix elements, if possible.

*Restrictions on the complexity of the problem*

Quadrupole matrix elements can be calculated up to $l = 500$ at most. Reasonable accuracy can be achieved only with $\xi/\eta \gtrsim 0.003$ (projectile's energy up to 170 times the excitation energy). For $\xi/\eta \lesssim 10^{-2}$, the accuracy of $10^{-7}$ cannot be acquired.

*References*

[1] K. Alder, A. Bohr, T. Huus, B. Mottelson and A. Winther, Rev. Mod. Phys. 28 (1956) 432.
[2] M. Samuel and U. Smilansky, Phys. Letters 28B (1968) 318.
[3] F. T. Baker and R. Tickle, Phys. Letters 32B (1970) 47.
[4] L. C. Biedenharn, J. L. McHale and R. M. Thaler, Phys. Rev. 100 (1955) 376.

COMPUTER PHYSICS COMMUNICATIONS 2 (1971) 470. NORTH-HOLLAND PUBLISHING COMPANY

# A NEW VERSION OF A PRINTER-PLOTTER ROUTINE

C. FRED MOORE
*Center for Nuclear Studies, University of Texas, Austin, Texas 78712, USA*

Received 29 July 1971

## PROGRAM SUMMARY

*Title of program*: PLOTT NEW VERSION

*Catalogue number*: ABOO

*Computer for which the program is designed and others upon which it is operable*

*Computer*: CDC 6600. *Installation*: University of Texas

*Operating system or monitor under which the program is executed*: UT1

*Programming languages used*: FORTRAN IV

*High speed store required*: 1811 words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 509

*Keywords descriptive of problem and method of solution*: General, Graphical Display, Printer Plotter.

*Reference to other published version of this program*:

*Catalogue number*: ABOI; *Title*: PLOTT; *Ref. in CPC*: 2 (1971) 55.

*Nature of physical problem*

This program solves the same problem as the routine PLOTT [1].

*Method of solution*

This is unaltered from that of ref. [1]. Some statements have been modified to make them more easily adaptable to other computers. In particular comments are included to indicate how to overcome problems concerned with character storage when converting the program to run on IBM 360 series computers. The test output is the same as printed in ref. [1].

*Reference*

[1] C. Fred Moore, Computer Phys. Commun. 2 (1971) 55.

## ERRATUM NOTICES

*Title of manuscript*: Relativistic self-consistent field program for atoms and ions

*Authors*: D. A. Liberman, D. T. Cromer and J. T. Waber

*Reference*: Computer Physics Communications 2 (1971) 107.

*Title of program*: HEX

*Catalogue number*: AAKB

*Title of manuscript*: Relativistic self-consistent field program for atoms and ions

*Authors*: D. A. Liberman, D. T. Cromer and J. T. Waber

*Reference* : Computer Physics Communications 2 (1971) 107.

*Title of program*: HEX

*Catalogue number*: AAKB

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 1–8. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR THE EXTRACTION OF BULK VISCOSITIES FROM SOUND ABSORPTION DATA

H. MORAAL
*Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada*

Received 2 July 1971

## PROGRAM SUMMARY

*Title of program*: SOUND ABSORPTION
*Catalogue number*: ABSA
*Computer for which the program is designed and others on which it is operable*
*Computer*: IBM 360/75. *Installation*: University of Waterloo Computing Centre
*Operating system or monitor under which the program is executed:* HASP/OS 360
*High speed store required*: 1600 words. *No. of bits in a word*: 32
*Is the program overlaid*? No
*No. of magnetic tapes required*: None
*What other peripherals are used ?* Card Reader; Line Printer
*No. of cards in combined program and test deck*: 320

*Keywords descriptive of problem and method of solution*: Atomic, Molecular, Plasma Physics, Sound Absorption, Rotational Relaxation, Bulk Viscosity, Least Squares Fitting

*Nature of physical problem*

Sound absorption measurements in polyatomic gases contain information about the energetically inelastic collisions which take place in the gas, i.e., those collisions in which the rotational state of one or both of the molecules changes. This fact manifests itself through the so-called bulk or volume viscosity. It is the purpose of this communication to describe a method whereby a reduced bulk viscosity may be obtained from the sound absorption data directly [1].

*Method of solution*

The unknown bulk viscosity enters the problem as a parameter in a determinantal equation. The program is designed so as to reconstruct the polynomial in two variables represented by this equation. This part of the program is useful whenever a polynomial is given in a determinantal form. In the case considered here, the two variables are the complex propagation constant, the imaginary part of which is proportional to the measured sound absorption coefficient, and the reduced collision frequency. The coefficients of the reconstructed polynomial are now functions of the unknown. These values are chosen in a systematic way so as to minimise the sum of the squares of the calculated differences of the theoretical and measured sound aborption coefficients.

*Typical running time*

The time depends on the number of experimental data available; for less than 50 data points the average is about 2–3 minutes.

*Unusual features of the program*

The experimental data can directly be used as input for the program.

*Reference*

[1] H. Moraal and F.R. McCourt, Z. Naturforsch., to be published.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 9–18. NORTH–HOLLAND PUBLISHING COMPANY

# CALCULATION OF ATOMIC ENERGY LEVEL VALUES

Leon J. RADZIEMSKI Jr., Kay J. FISHER and David W. STEINHAUS
*Los Alamos Scientific Laboratory of the University of California, Los Alamos, New Mexico 87544, USA*

and

Aaron S. GOLDMAN
*University of Nevada, Las Vegas, Las Vegas, Nevada 89109, USA*

Received 7 October 1970
Revised manuscript received 27 July 1971

## PROGRAM SUMMARY

*Title of program*: LEVEL

*Catalogue number*: AAKD

*Computer*: Control Data 6600. *Installation*: Los Alamos Scientific Lab.

*Operating system*: Scope 3.1.2 (LASL modified)

*Programming language*: FORTRAN IV

*High speed store required*: 55 000 words. *No of bits in a word*: 60

*Is the program overlaid?* Yes

*No. of magnetic tapes required*: 4 may be used for input data, intermediate storage and to store the results

*What other peripherals are used?* Disk (in lieu of tapes); Extended Core Storage (disk may be substituted); Card Reader; Printer

*No. of cards in combined program and test deck*: 2521

*Keywords*: Atomic, Energy Level, Least Squares Solution, Matrix Inversion, Isotope Shift, Spectra.

*Nature of the physical problem*

An atomic energy level array consists of two sets of energy levels of different parity and transitions between them (we exclude transitions within sets). There are wide variations in the accuracies of the wave number values of observed classified transitions, and usually many more observed transitions than energy levels. The problem is to determine the best values for the levels and their uncertainties. The uncertainties are very important because these are used to determine the accuracies of wave numbers computed from the energy levels. Calculation of level isotope shifts can also be made since this is a trivial variation of the level calculation problem [1, 2].

*Method of solution*

The normal equations obtained from the least squares formulation are partitioned to reduce the size of the matrix to be inverted to the magnitude of the smaller set of energy levels. The variance-covariance matrix is used to compute corrections to the values of the energy levels and to compute variances on the levels and on the computed wave numbers. The method of inversion produces results with round-off error beyond the significance of the data involved with this kind of physical problem. Only half of the symmetric matrix is stored, and the inverse is stored in the same location so storage requirements are minimized.

*Restrictions on the complexity of the problem*

High speed core storage of 64 000 words limits the number of levels on the small side to 285 and the number of classifications to 19 000.

*References*

[1] L. J. Radziemski Jr., K. J. Fisher and D. W. Steinhaus, Los Alamos Scientific Laboratory Report LA-4402 (1970).
[2] K. L. Vander Sluis, J. Opt. Soc. Am. 56 (1969) 1600.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 19–21. NORTH-HOLLAND PUBLISHING COMPANY

# WAVE NUMBER CALCULATION FROM LEAST-SQUARES LEVEL VALUES

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and

Aaron S. GOLDMAN
*University of Nevada, Las Vegas, Las Vegas, Nevada 89109, USA*

Received 7 October 1970

## PROGRAM SUMMARY

*Title of program:* CALOR

*Catalogue number:* AAKE

*Computer:* Control Data 6600. *Installation:* Los Alamos Scientific Lab.

*Operating system:* Scope 3.1.2. (LASL modified)

*Programming language:* FORTRAN IV

*High speed store required:* 51 000. *No. of bits in a word:* 60

*Is the program overlaid?* No

*No. of magnetic tapes required:* One

*What other peripherals are used?* Card Reader; Printer; and 40 000 Words of Extended Core Storage

*No. of cards in combined program and test deck:* 309

*Keywords:* Atomic, Energy Level, Least Squares Solution, Wave Number.

*Nature of the physical problem*

Wave numbers are calculated from least-squares level values. These are more accurate than experimentally determined wave numbers.

*Method of solution*

This code takes the output of the LEVEL [1] code (previous paper) and calculates wave numbers and their variances.

*Restrictions on the complexity of the problem*

Only allowed transitions ($\Delta J = 0, \pm 1$) can be calculated.

*Typical running time*

0.35 sec for 15 000 wave numbers.

*Reference*

[1] L.J.Radziemski Jr., K.J.Fisher, D.W.Steinhaus and A.S. Goldman, Computer Phys. Commun. 3 (1972) 9.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 22–30. NORTH-HOLLAND PUBLISHING COMPANY

# HARTREE–FOCK NUCLEAR CALCULATIONS WITH GAUSSIAN POTENTIALS

J.F. ALLARD, A. ABZOUZI and B. HOUSSAIS
*Institut d'Etudes Nucléaires B.P. 1147 Alger, Algerie*

Received 4 May 1971

## PROGRAM SUMMARY

*Title of program:* (32 characters maximum): HARFOCK

*Catalogue number:* ABGD

*Computer for which the program is designed and others upon which it is operable*

*Computer:* IBM 360/40. *Installation:* Ministère de l'Education Nationale (Alger)

*Operating system or monitor under which the program is executed:* DOS

*Programming languages used:* FORTRAN IV

*High speed store required:* 16 K. *No. of bits in a word:* 32

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck:* 619

*Keywords descriptive of problem and method of solution:* Nuclear, Schrödinger Equation, Ground State Energies, Excitation Energies, Deformations, Hartree–Fock, Self-consistent Field.

*Nature of physical problem*

The program is designed to calculate wavefunctions and energies of nucleons up to the 2s 1d shell using the Hartree–Fock method.

The two-body interaction is a sum of two gaussian potentials with spin, isospin and space exchange terms. The kinetic energy of the centre of mass $T_{\mathrm{cm}}$ is subtracted but the Coulomb interaction is neglected.

A one-body potential $C\, l \cdot s$ may be added to the kinetic energy.

A cartesian harmonic oscillator basis is used, with independent $\omega_x$, $\omega_y$, $\omega_z$ constants for each of the coordinate axes.

*Method of solution*

The program calculates a self-consistent nuclear field and determines orbital energies and wavefunctions of the nucleus considered [1, 2].

*Restrictions on the complexity of the problem*

The basis used for the description of the spacial part of the wavefunction includes the ten basis elements of the 1s, 1p, 2s 1d deformed shells and therefore the program may be used only for light nuclei. Orbitals must be eigenstates of parity but they may have no other symmetry.

*References*

[1] D.M.Brink and E.Boeker, Nucl. Phys. A91 (1967) 1.
[2] E.Boeker, Nucl. Phys. A91 (1967) 27.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 31–35. NORTH-HOLLAND PUBLISHING COMPANY

# DIRECT COMPUTATION OF THE MAGNETIC SHELL PARAMETER

G.KLUGE
*ESOC*, 6100 *Darmstadt, Germany*

Received 18 January 1971

## PROGRAM SUMMARY

*Title of program*: SHELL

*Catalogue number*: AAEA

*Computer*: IBM/360–65. *Installation*: ESOC, Darmstadt

*Operating system or monitor under which the program is executed*: /360–OS

*Programming languages used*: FORTRAN IV

*High speed store required*: < 2500 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* None

*No. of cards in combined program and test deck*: 432

*Keywords descriptive of problem and method of solution*: Geophysics, Space Science, Geomagnetic Field, Trapped Radiation, Field Lines, Multipole Expansion, Perturbation Method

*Nature of physical problem*

The "magnetic coordinates" $B$ and $L$ are adiabatic invariants of the motion of charged particles trapped in the magnetic field of the earth and, therefore, convenient for correlating measured particle fluxes.

*Method of solution*

A perturbation approach is used for the integration of the differential equations for the field lines.

*Typical running time*

Average 80 msec per value.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 36–41. NORTH-HOLLAND PUBLISHING COMPANY

# NUMERICAL FITS FOR THE GEOMAGNETIC SHELL PARAMETER

G. KLUGE and K.G. LENHART
*ESOC*, 6100 *Darmstadt, Germany*

Received 18 January 1971

## PROGRAM SUMMARY

*Title of program*: INTEL

*Catalogue number*: AAEB

*Computer*: IBM/360–65. *Installation*: ESOC, Darmstadt

*Operating system or monitor under which the program is executed*: /360–OS

*Programming languages used*: FORTRAN-IV

*High speed store required*: < 2500 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* None

*No. of cards in combined program and test deck*: 518

*C.P.C. Library subprogram used*:

*Catalogue number*: AAEA; *Title*: SHELL; Ref. in CPC: 3 (1972) 31.

*Keywords descriptive of problem and method of solution*: Geophysics, Space Science, Geomagnetic Field, Trapped Radiation, Fourier Series, Interpolation

*Nature of physical problem*

The "magnetic coordinates" $B$ and $L$ are adiabatic invariants of the motion of charged particles trapped in the magnetic field of the earth and, therefore, convenient for correlating measured particle fluxes.

*Method of solution*

The shell parameter is represented by Fourier series and interpolation. Several hundred parameters are fitted to data obtained from direct computation. The rms error of the fit is about 0.05%.

*Typical running time*

12 msec to compute $B$ and $L$.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 42–52. NORTH-HOLLAND PUBLISHING COMPANY

# TRAJECTORY CALCULATIONS FOR THE REACTION K + HBr → KBr + H IN THE eV-REGION

A. van der MEULEN

*FOM-Instituut voor Atoom- en Molecuulfysica, Amsterdam, The Netherlands*

Received 22 July 1971

## PROGRAM SUMMARY

*Title of program*: CLASSICAL TRAJECTORIES 324

*Catalogue number*: AAGI

*Computer for which the program is designed and others on which it is operable*

*Computer*: NV Philips El-X8. *Installation*: Mathematisch Centrum, Amsterdam, The Netherlands

*Operating system or monitor under which the program is executed*: MILLI; MCALL

*Programming languages used*: ALGOL 60

*High speed store required*: 3660 words. *No. of bits in a word*: 54

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Paper Tape Reader; Paper Tape Punch; Printer

*No. of lines in combined program and test deck*: 325

*Keywords descriptive of problem and method of solution*: Atomic, Molecular, Chemical Reaction, 3-Dimensional, Classical, Trajectory, Second Order Differential Equations, Runge–Kutta–Zonneveld, Stepsize Control, Potential Energy Variation, Array Elements

*Nature of physical problem*

A series of three-dimensional classical kinematic computer trajectory calculations have been made on the exothermic exchange reaction K + HBR → KBr + H, $\Delta H = -0.206$ eV. The total reaction cross section for the formation of KBr, as well as the angular distribution of non-reactive scattered K was obtained as a function of initial relative kinetic energy, which was varied between 0.03 and 30 eV.

*Method of solution*

By means of a suitable canonical transformation the 18 equations of motion could be reduced to a system of 6 linear second order coupled differential equations: $\ddot{Q}_i = -\partial V/\partial Q_i$, $i = 1, 2, ..., 6$; $V$ being the total potential energy and $Q_i$ the generalized coordinates. The integration of this system is performed by means of a specially adapted version of the Runge–Kutta–Zonneveld RK3n-procedure, with variable stepsize.

*Typical running time*

The evaluation of one complete trajectory takes about 10 sec, if the following conditions are satisfied:

(i) conservation of energy better than 0.1%;
(ii) initial distance between K and the centre of mass of HBr equals 8 Å;
(iii) the integration is terminated if at least 2 of the 3 interatomic distances H–Br, K–Br and K–H exceed 5, 8 and 8.5 Å respectively.

*Restrictions on complexity*

The program can easily be modified to accept potential energy functions of any analytic form, rather than the L.E.P.S. expression used in this work.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 53–60. NORTH-HOLLAND PUBLISHING COMPANY

# GENERALIZED TRANSFORMATION BRACKETS FOR THE HARMONIC OSCILLATOR FUNCTIONS

M. SOTONA and M. GMITRO
*Nuclear Research Institute, Řež (Prague), Czechoslovakia*

Received 7 September 1971

## PROGRAM SUMMARY

*Title of program* (*32 characters maximum*): OSCILLATOR BRACKETS

*Catalogue number*: ABGH

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 7040. *Installation*: Computing Laboratory for Economical Planning, Prague

*Operating system or monitor under which the program is executed*: IBSYS

*Programming languages used*: FORTRAN IV

*High speed store required*: 3003 words. *No. of bits in a word*: 36

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck:* 412

*Keywords descriptive of problem and method of solution*: Nuclear, Nuclear Spectra, Nuclear Structure, Nuclear Reaction, Cluster Model, Shell Model, Matrix Element, Talmi Coefficient, Brody–Moshinsky Bracket, Angular Momentum, Harmonic Oscillator.

*Nature of the physical problem*

The program calculates the transformation coefficient in the expansion of two coupled harmonic oscillator wavefunctions (for particles 1 and 2) into coupled pairs of relative and centre-of-mass functions. It will thus be of general use in almost any calculation using harmonic oscillator bases.

*Method of solution*

The formula used for computation is essentially of a recursive type. It starts with the $l = 0$ case and is therefore especially suited for the brackets with one small angular momentum as required in modern nuclear structure calculations with realistic nucleon–nucleon potentials.

*Restrictions on the complexity of the problem*

The only restrictions come from the core area assigned to store logarithms of factorials and gamma functions calculated once and for all at the beginning of execution. Since the core requirements are very modest an enlargement of the corresponding arrays is always possible.

*Typical running time*

The running time strongly depends on the smallest angular momentum that appears in a given coefficient and on the nodal quantum numbers. Only the relative angular momenta $l = 0, 1$ and 2 are usually needed, then the average time to calculate one such coefficient is about 50, 100, 200 msec respectively on an IBM 7040. See also table 1 of the long write-up.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 61–68. NORTH-HOLLAND PUBLISHING COMPANY

# A FORTRAN PROGRAM FOR THE COMPUTATION OF THE GENERALIZED TALMI COEFFICIENTS *

O. ZOHNI **
*International Centre for Theoretical Physics, 34100 Trieste, Italy*

Received 1 September 1971

## PROGRAM SUMMARY

*Title of program*: TALMI

*Catalogue number*: ABGG

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 7044. *Installation*: Centro di Calcolo dell'Università di Trieste

*Operating system or monitor under which the program is executed*: IBSYS

*Programming language used*: FORTRAN

*High speed store required*: 5222 words. *No. of bits in a word*: 36

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 964

*Keywords descriptive of problem and method of solution*: Nuclear, Nuclear Spectra, Nuclear Structure, Nuclear Reaction, Cluster Model, Shell Model, Matrix Element, Talmi coefficient, Brody–Moshinsky Bracket, Angular Momentum, Harmonic Oscillator.

*Nature of the physical problem*

The program calculates the generalized Talmi coefficients $\langle n_1 l_1, n_2 l_2 : \lambda | \mu_1 \mu_2 | NL, nl : \lambda \rangle$ defined in ref. [1] and used to obtain the centre-of-mass (c.m.) and relative wavefunctions of two particles having different masses $\mu_1$ and $\mu_2$ moving in a harmonic oscillator potential. With these coefficients, it is easy to separate the c.m. motion of a group of nucleons in the shell model as well as of nucleon clusters in the cluster model of nuclei [2].

*Method of solution*

The program makes use of the formula given in ref. [1]. This formula includes sums over a relatively large number of indices whose values are governed by a comparable number of selection rules. To calculate a Talmi coefficient, the selection rules are appropriately set up, and then the sums over the different indices are computed in a straightforward way by a nest of DO loops.

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* A preliminary version of this FORTRAN code was designed and operated on the ICL 1905 E Computer (1900 series) installed at the Scientific Computer Centre, Cairo University.

** On leave from Physics Department, Faculty of Science, Cairo University, Giza, UAR.

*Typical running time*

The time required to calculate a Talmi coefficient depends upon the values of its arguments. For values of arguments ranging from 0 to 4, the execution time of a coefficient varies from 0.3 to 1.5 seconds on the IBM 7044.

*References*

[1] Yu.F. Smirnov, Nucl. Phys. 27 (1961) 177.

[2] Yu.A. Kudeyarov, Z. Matthies, V.G. Neudachin and Yu.F.Smirnov, Nucl. Phys. 65 (1965) 529.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 73–87. NORTH-HOLLAND PUBLISHING COMPANY

# COULOMB FUNCTIONS IN ENTIRE $(\eta, \rho)$ - PLANE

C. BARDIN, Y. DANDEU, L. GAUTHIER, J. GUILLERMIN
T. LENA and J.-M. PERNET
*Centre d'Etudes Nucléaires de Saclay, 91 Gif-sur-Yvette, France*

and

H.H. WOLTER† and T. TAMURA
*Center for Nuclear Studies††, Universtiy of Texas,*
*Austin, Texas, USA*

Received 9 November 1971

## PROGRAM SUMMARY

*Title of program* : COULOM FOR REAL ENERGY

*Catalogue number* : ABOQ

*Computer for which the program is designed and others upon which it is operable*

*Computer* : CDC 6600. *Installation* : Univ. of Texas Computation Center

*Operating system or monitor under which the program is executed* : UT-2

*Programming languages used* : ASA FORTRAN

*High speed store required* : 23 K. *No. of bits in a word* : 60

*Is the program overlaid* ? No

*No. of magnetic tapes required* : None

*What other peripherals are used* ? Card Reader; Printer

*No. of cards in combined program and test deck* : 1073

*Keywords descriptive of problem and method of solution* : Nuclear, Schrödinger Eq., Reactions, Scattering, Heavy Ion, Wave-function, Coulomb, Potential, Complex Gamma Function, MacLaurin Expansion, Taylor Expansion, Asymptotic Expansion, Chebychev Expansion, Clenshaw Expansion, Riccati Method, Confluent Hypergeometric Functions.

*Nature of physical problem*

The subroutine COULOM calculates the regular and irregular Coulomb functions $F_l(\eta, \rho)$ and $G_l(\eta, \rho)$ and their derivatives for real positive energy in the whole $(\eta, \rho)$ -plane $(-500 \leqslant \eta \leqslant 500, \rho \geqslant 0)$ with a uniformly high accuracy. This program will be useful, e.g., for the nuclear scattering and reaction calculations involving heavy projectiles, when $\rho$ is no longer very large compared with $\eta$. It thus supplements existing programs that usually require $\rho \gg \eta^2$.

*Method of solution*

The behaviour of the Coulomb functions in the $(\eta, \rho)$-plane varies widely. Of special importance is the transition line $\rho = 2\eta$, where for $l$=0 the character changes from exponential to oscillatory. Different forms of expansions are chosen in different regions of the $(\eta, \rho)$-plane in a way similar but not identical to that of Froberg [1]. These methods include Maclaurin expansion, Taylor expansion, asymptotic expansion, Chebychev expansion and Riccati method. A subroutine calculates the complex gamma function and its logarithmic derivative. The Coulomb functions for $l > 0$ are calculated by using recursion relations employing a new technique recently proposed by Wills [2].

---

† Supported by Heinrich-Hertz-Stiftung des Landes Nordrhein-Westfalen, Germany.

†† Supported in part by the U.S. Atomic Energy Commision.

*Restrictions on the complexity of the problem*

The parameters $\eta$ and $\rho$ have to be real. For complex $\eta$ and $\rho$, due to complex energy, see ref. [3].

*References*

[1] C.E. Fröberg, Rev. Mod. Phys. 27 (1955) 399.
[2] J.G. Wills, J. Comp. Phys., to be published.
[3] T.Tamura and F. Rybicki, Computer Phys. Commun. 1 (1969) 25.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 88–117. NORTH-HOLLAND PUBLISHING COMPANY

# GROUP-THEORETICAL ANALYSIS OF LATTICE VIBRATIONS[†]

T.G. WORLTON
*Argonne National Laboratory, Argonne, Illinois 60439, USA*

and

J.L. WARREN
*Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87544, USA*

Received 18 October 1971

## PROGRAM SUMMARY

*Title of program*: GROUP THEORY OF LATTICE DYNAMICS

*Catalogue number*: ACMI

| *Computer:* | | *Installation:* | |
|---|---|---|---|
| *Computer:* | IBM 360/75 | *Installation:* | Argonne Nat'l. Lab. |
| | CDC 6600 | | Los Alamos Sci. Lab. |

*Operating system or monitor under which the program is executed*: IBM System 360 MVT, Release 19; Scope 3.1.2. (modified by LASL) for CDC

*Programming laguages used*: FORTRAN IV

*High speed store required*: 36000 words. *No. of bits in a word*: 32 (60 CDC)

*Is the program overlaid* ? No

*No. of magnetic tapes required*: None

*What other peripherals are used* ? Printer; Card Reader

*No. of cards in combined program and test deck*: 1619

*Keywords descriptive of problem and method of solution*: Solid State, Lattice Dynamics, Group Theory, Phonons, Symmetry, Dispersion Curves, Dynamical Matrix, Multiplier Representation Method.

*Nature of physical problem*

The program block-diagonalizes the dynamical matrix characterizing lattice vibrations of solids, constructs symmetry coordinates, and labels these coordinates with the irreducible representations of the symmetry group.

*Method of solution*

Using a reducible multiplier representation of the point group of the wavevector, projection operators are constructed. These give symmetry coordinates which are used to block diagonalize the dynamical matrix.

*Restrictions on the complexity of the problem*

The program is dimensioned for up to 10 atoms per unit cell; by changing a dimension statement, it should handle up to 20 atoms per unit cell. For certain low-symmetry crystals in the trigonal and hexagonal systems the symmetry reduction of the dynamical matrix will be incomplete because of complicated relations between elements.

---

[†] Based on work performed under the auspices of the US Atomic Energy Commission.

*Unusual features of the program*

The program also constructs the point group of the crystal, determines Brillouin-Zone boundaries and optical modes exhibiting infrared and Raman activity. Effects of time-reversal invariance are included.

*References*

[1] A.A. Maradudin and S.H. Vosko, Rev. Mod. Phys. 40 (1968) 1;

[2] J.L. Warren, Rev. Mod. Phys. 40 (1968) 38;

[3] O.V. Kovalev, Irreducible representations of the space groups (Gordon and Breach, New York, 1965).

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 118–129. NORTH-HOLLAND PUBLISHING COMPANY

# DIFFERENTIAL CROSS SECTIONS FOR ELECTRIC QUADRUPOLE COULOMB EXCITATION I *

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and

A. B. LOPEZ-CEPERO ***
*University of Texas, Austin, Texas, USA*

Received 10 August 1971

## PROGRAM SUMMARY

*Title of program*: DXS1

*Catalogue number*: ABQE

*Computer for which the program is designed and others upon which it is operable*

*Computer*: IBM 360/75. *Installation*: Triangle University Computation Center, Research Triangle Park, North Carolina

*Operating system or monitor under which the program is executed*: OS-360-MVT

*Programming languages used*: FORTRAN-IV (G)

*High speed store required*: 35 000 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1172

*Keywords descriptive of problem and method of solution*: Nuclear, Electric Quadrupole, Coulomb Excitation, Differential Cross Section, Inelastic Scattering, Radial Coulomb Integrals, Finite Sums.

*Nature of the physical problem*

The program calculates the differential cross section for inelastic scattering of a structureless charged particle through E2 excitation of a point nucleus. It is assumed that all nuclear effects can be ignored.

*Method of solution*

The numerical calculation closely follows the well-known quantum-mechanical theory of Coulomb excitation [1, 2] in the distorted wave Born approximation. The target and projectile are assumed to be point particles. Radical integrals are calculated in the long wavelength (of the transferred photon) limit.

*Restrictions on the complexity of the problem*

The calculation is non-relativistic and in the center of mass coordinates. In spite of the program's capability to consider up to 300 partial waves, even that may not provide good results with a combination of very small energy loss and small scattering angles.

---

* Research supported in part by the National Science Foundation and the Army Research Office (Durham).

** Present address: Davidson County Community College, Lexington, North Carolina, USA.

*** Work done at Duke University.

### *Unusual features of the program*

The capacity for considering up to 300 partial waves is necessary to get reliable results for small angle scattering. The spherical harmonics are calculated by a recursion relation that is very stable for high angular momenta [3], as are the techniques for computing the Clebsch–Gordan and Racah coefficients. The finite-sum method [4] is used for calculating the radial integrals. This methods is remarkably fast and stable with respect to errors; at present there are no available codes for Coulomb excitation that incorporate this method.

### *Typical running time*

In the IBM 360/75 the program takes about 52 seconds to compile and the running time depends on the number of partial waves used. Typically for about 60 partial waves it takes about 2 minutes to calculate the radial integrals and an extra 15 seconds for each angle. Running time increases significantly with increase in the number of partial waves used.

### *References*

[1] K. Alder, A. Bohr, T. Huus, B. Mottelson and A. Winther, Rev. Mod. Phys. 28 (1956) 432.

[2] L. C. Biedenharn and P. J. Brussaard, Coulomb excitation (Clarendon Press, Oxford, 1965).

[3] S. L. Belousov, Tables of normalized associated Legendre polynomials (MacMillan, New York, 1962).

[4] M. Goldstein, R. M. Thaler and L. C. Biedenharn, A tabulation of the radial Coulomb integrals (*n, m, l*), LASL Report LA-2106 (1957).

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 130–135 . NORTH-HOLLAND PUBLISHING COMPANY

# FIELD AND FIELD GRADIENT INTEGRALS BASED ON GAUSSIAN TYPE ORBITALS

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*Laboratory of Atomic Physics, The University of Electro-Communications, Chofu-shi, Tokyo, Japan*

Received 22 October 1971

## PROGRAM SUMMARY (FIELD INTEGRAL)

*Title of program*: FIELD

*Catalogue number*: ABYB

*Computer for which the program is designed and others upon which it is operable*

*Computer*: HITAC 5020E. *Installation*: Computer Centre, University of Tokyo, Tokyo, Japan

*Operating system or monitor under which the program is executed*: HIJOB

*Programming languages used*: FORTRAN IV

*High speed store required*: 9253 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 568

*Keywords descriptive of problem and method of solution*: Quantum Chemistry, Field Integral, Molecular Integral, Gaussian Type Orbital, Combined Gaussian Type Orbital, Contracted Gaussian Orbital.

*Nature of physical problem*

The function subprogram FIELD with associated subroutines FGAMA and FTABL computes the field integral based on combined [1] or contracted [2] gaussian-type orbitals (CGTO). The field integral is defined by [3]

$$\int \phi(A, l_1, m_1, n_1) F_C \phi(B, l_2, m_2, n_2) \mathrm{d}V,$$

where $F_C$ is the field operator written as

$F_C = x_C/r_C^3$, $y_C/r_C^3$, or $z_C/r_C^3$, and $\phi(A, l, m, n)$ is the CGTO.

*Method of solution*

The value of the integral is analytically evaluated by the method of ref. [3].

*Restrictions of the complexity of the problem*

The sum of the quantum numbers $l$, $m$, and $n$ of a CGTO appearing in the integral is restricted to 0, 1 or 2 (i.e., $0 \leqslant l+m+n \leqslant 2$).

*Unusual features of the program*

The program FIELD should not be used before calling the subroutine FTABL.

*Typical running time*

The construction of the table of $F$-functions [3] requires four seconds. The computation of the 39 integrals over the six-term CGTO's of various quantum numbers takes about one second on the HITAC 5020E.

*References*

[1] H. Taketa, S. Huzinaga and K. O-ohata, J. Phys. Soc. Japan 21 (1966) 2313.
[2] D. Davis and E. Clementi, J. Comput. Phys. 1 (1966) 223.
[3] O. Matsuoka, Intern. J. Quantum Chem. 5 (1971) 1.

## PROGRAM SUMMARY (FIELD GRADIENT INTEGRAL)

*Title of program*: FGRAD

*Catalogue number*: ABYC

*Computer for which the program is designed and others upon which it is operable*

*Computer*: HITAC 5020E. *Installation*: The Computer Centre, University of Tokyo, Tokyo, Japan

*Operating system or monitor under which the program is executed*: HIJOB

*Programming languages used*: FORTAN IV

*High speed store required*: 9553 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 638

*Keywords descriptive of problem and method of solution*: Quantum Chemistry, Field Gradient Integral, Molecular Integral, Gaussian Type Orbitals, Combined Gaussian Type Orbital, Contracted Gaussian Orbital.

*Nature of physical problem*

The function subprogram FGRAD with associated subroutines FGAMA and FTABL computes the field gradient integral based on combined [1] or contracted [2] gaussian type orbitals (CGTO). The field gradient integral is defined by [3]

$$\int \phi(A, l_1, m_1, n_1) G_C \phi(B, l_2 m_2, n_2) \mathrm{d}V ,$$

where $G_C$ is the field gradient operator written as

$$G_C = (3x_C^2 - r_C^2)/r_C^5, (3y_C^2 - r_C^2)/r_C^5, \text{ or } (3z_C^2 - r_C^2)/r_C^5 ,$$

and $\phi(A, l, m, n)$ is the CGTO.

*Method of solution*

The value of the integral is analytically evaluated by the method of ref. [3].

*Restrictions on the complexty of the problem*

The sum of the quantum numbers $l$, $m$, and $n$ of a CGTO appearing in the integral is restricted to 0, 1, or 2 (i.e., $0 \leqslant l+m+n \leqslant 2$).

*Unusual feature of the program*

The program FGRAD should not be used before calling the subroutine FTABL.

*Typical running time*

The construction of the table of $F$-functions [3] requires four seconds. The computation of the 39 integrals over six-term CGTO's of various quantum numbers takes about two seconds on the HITAC 5020E.

*References*

[1] H. Taketa, S. Huzinaga and K.O-ohata, J. Phys. Soc. Japan 21 (1966) 2313.
[2] D. Davis and E. Clementi, J. Comput. Phys. 1 (1966) 223.
[3] O. Matsuoka, Intern. J. Quantum Chem. 5 (1971) 1.

COMPUTER PHYSICS COMMUNICATION 3 (1972) 136–154. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR THE GENERATION OF ARTIFICIAL BUBBLE CHAMBER EVENTS

J. BETTELS and P. DODD*
*CERN, 1211 Geneva 23, Switzerland*

Received 6 May 1971

## PROGRAM SUMMARY

*Title of program*: GAT

*Catalogue number*: AAUC

*Computer for which the program is designed and others on which it is operable*:

| *Computer*: | | *Installation*: |
|---|---|---|
| CDC | 6000 series. | CERN |
| CDC | 3200 | CERN |
| IBM | 360/50 | Bergen, Norway |
| IBM | 360/75 | Saclay, France |
| IBM | 360/91 | Munich, Germany |
| CII | 10070 | Aachen, Germany |
| UNIVAC | 1108 | Orsay, France |

*Programming language used*: ASA FORTRAN IV

*High speed store required*: 19100 words, 6000 of which is data store. *No. of bits in a word*: 60 on CDC 6600

*Is the program overlaid?* No

*No. of magnetic tapes required*: One

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 4516

*Keywords descriptive of problem and method of solution*: Nuclear, High Energy, Particle Physics, Bubble Chambers, Artificial Events.

*Nature of physical problem*

To simulate the output of bubble chamber measurements, with particular reference to the new large bubble chambers.

*Method of solution*

From a set of starting parameters a track is propagated by solving the equations of motions using a Runge-Kutta technique, allowing for energy-loss, radiation-loss and multiple scattering. For each event a beam particle with given starting parameters and interaction length, is traced until it interacts. A choice is made among a set of permitted interaction channels, and the initial parameters of the appropriate secondary tracks are calculated, assuming Fermi phase-space statistics. These secondary tracks are then propagated until they leave the chamber volume, stop or interact.

All calculated track points are then transformed onto a nominal film plane. Some of these transformed points are then selected as "measurements" according to various criteria specified by the user. The usual method is to select points equidistant along the transformed track.

*Restrictions on the complexity of the problem*

The present program has a maximum of 10 tracks and 20 vertices per event. Neutral particles from secondary interactions are not treated. Both these restrictions can be removed by minor alterations to the coding.

---

* Present address: The Computer Centre, The University of Birmingham, Birmingham B15 2TT, UK.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 155–158. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTER GENERATED WEYL GROUPS

Robert E. BECK
*Villanova University, Villanova, Pennsylvania 19085, USA*

and

Bernard KOLMAN
*Drexel University, Philadelphia, Pennsylvania 19104, USA*

Received 11 August 1971

## PROGRAM SUMMARY

*Title of program:* WEYL GROUP
*Catalogue number*: ACRA
*Computer for which the program is designed and others upon which it is operable:*
*Computer:* IBM 360/75. *Installation:* University of Pennsylvania
*Operating system or monitor under which the program is executed:* HASP-II
*Programming languages used:* FORTRAN IV
*High speed store required:* 40213 words. *No. of bits in a word:* 32
*Is the program overlaid?* No
*No. of magnetic tapes required:* None
*What other peripherals are used?* Card Reader; Line Printer
*No. of cards in combined program and test deck:* 607

*Keywords descriptive of problem and method of solution:* General, Weyl Group, Lie Algebra, Reflection Group, Symmetry Group, Coset Representation, Equivalent Particles.

*Nature of physical problem*
To generate the Weyl group of a complex simple Lie algebra and store in a high speed memory.

*Method of solution*
The symmetric group $S_n$ is first generated by finding coset representatives of $S_{n-1}$ in $S_n$. Coset representatives of $S_n$ in the Weyl group are then generated.

*Restrictions on the complexity of the problem*
The program handles all Lie algebras of rank $\leqslant 4$.

*Typical running time*
0.03 sec for $B_2$, 0.19 sec for $C_3$, 0.81 sec for $D_4$.

*Unusual features of the program*
Group is stored in a manner that makes it easily used in the computation of characters of irreducible representations of simple Lie algebras on a computer.

*Reference*
[1] R. E. Beck and B. Kolman, J. Comp. Phys. 7 (1971) 346.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 173–179. NORTH-HOLLAND PUBLISHING COMPANY

# THE CALCULATION OF ABSORPTION AND ELASTIC CROSS SECTIONS USING THE OPTICAL POTENTIAL

Arthur C. ALLISON

*Smithonian Astrophysical Observatory, Cambridge, Massachusetts 02138, USA*

Received 3 January 1972

## PROGRAM SUMMARY

*Title of program*: SCATTERING BY COMPLEX POTENTIAL

*Catalogue number*: AACF

*Computer*: CDC 6400. *Installation*: Smithsonian Astrophysical Observatory, Cambridge, Massachusetts 02138, USA

*Operating system*: SCOPE 3/35

*Programming languages used*: FORTRAN

*High speed store required*: 12500 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 625

*Keywords*: Atomic, Potential, Complex Potential, Optical Model, Optical Potential, Schrödinger Equation, Numerov, Scattering, Absorption, Cross Section, Phase Shift.

*Nature of physical problem*

The absorption of particles by a centre of force may be represented by introducing a complex potential [1]. The absorption and elastic cross sections are given in terms of the real and imaginary parts of the phase shift obtained from the solution of the Schrödinger equation with a complex potential.

*Method of solution*

This program is similar to one published earlier by Smith [2] that also allows scattering by a complex potential to be studied. The present program permits greater flexibility in the form of the potential and also uses an improved Numerov scheme [3] for integrating the differential equations.

*Restrictions on the complexity of the problem*

The program can be easily modified to accept non-Coulomb potential energy functions of any form rather than the complex spherical well that is used in this version.

*Typical running time*

The time depends critically on the number of points in the integration mesh. For the test case, which required two hundred points, three complex phases were generated each second.

*Unusual features of program*

The computation time of the numerical integration is halved because of the symmetry of the problem and the use of the iterative Numerov method [3].

*References*

[1] N.F. Mott and H.S.W. Massey, The theory of atomic collisions, 3rd. Ed. (Clarendon Press, Oxford, 1965) p. 184.
[2] W.R. Smith, Computer Phys. Commun. 1 (1969) 106.
[3] A.C. Allison, J. Comp. Phys. 6 (1970) 378.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 197–220. NORTH-HOLLAND PUBLISHING COMPANY

# CLASSICAL RELATIVE MOTION OF 2 PARTICLES (EVAR EDITION 02)

D. BANKS, I.C. PERCIVAL and J.McB. WILSON
*Department of Physics, University of Stirling, Stirling, UK*

Received 18 October 1971

## PROGRAM SUMMARY

*Title of program*: EVAR EDITION 02

*Catalogue number*: ACRB

*Computer*: ELLIOT 4130. *Installation*: University of Stirling, Stirling, UK

*Operating system*: ENL 26

*Programming language used*: ASA FORTRAN

*High speed storage required*: 6000 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 3828

*Reference to other published version of this program*: Catalogue number: ACQT; Title: EVAR; Ref. in CPC: 2 (1971) 114.

*Keywords*: Atomic, Astrophysics, Molecular, Classical, Coulomb, Diatomic, Euler, Forces, Frame, Gravitational, Hydrogen, Interatomic, Kepler, Newtonian, Orbit, Particle, Runge–Kutta, Scattering, State, Vibrational.

*Nature of the physical problem*

This paper describes an updating of the package EVAR [1].

*Reference*

[1] D. Banks, I.C. Percival and J.McB. Wilson, Computer Phys. Commun. 2 (1971) 114.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 221–239. NORTH–HOLLAND PUBLISHING COMPANY

# CLASSICAL MOTION OF 2 PARTICLES (EVA2 EDITION 01)

D. BANKS, I.C. PERCIVAL and J. McB. WILSON
*Department of Physics, University of Stirling, Stirling, UK*

Received 18 October 1971

## PROGRAM SUMMARY

*Title of program*: EVA2 EDITION 01

*Catalogue number*: ACRC

*Computer*: ELLIOT 4130. *Installation*: University of Stirling, Stirling, UK

*Operating system or monitor under which the program is executed*: ENL 26

*Programming language used*: ASA FORTRAN

*High speed storage required*: 2000 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1451

*CPC Library subprogram used*:

*Catalogue Number*: ACRB; *Title*: EVAR EDITION 02; Ref. in CPC: 3 (1972) 195

*Keywords*: Atomic, Molecular, Astrophysics, Classical, Coulomb, Diatomic, Euler, Forces, Frame, Gravitational, Hydrogen, Interatomic, Kepler, Newtonian, Orbit, Particle, Representation, Runge–Kutta, Scattering, State, Vibrational.

*Nature of physical problem*

Flexible representation of the classical motion of two particles interacting through a general central force.

*Method of solution*

A general terminology of states, frames and representations is introduced which allows changes from one state or frame to another to be defined. The frame changes are analytic. The state changes are, in general, made by transforming to the centre of mass representation and using the package EVAR EDITION 02 [1].

*Restrictions on the complexity of the problem*

Limited to central forces.

*Typical running time*

This depends on the form of the potential, the boundary conditions and the integration time specified.

*Unusual features of the program*

The main program is only a driver program for the test run, the sub-programs of the package being more important.

*Reference*

[1] D. Banks, I.C. Percival and J. McB. Wilson, Computer Phys. Commun. 3 (1972) 195.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 240–255. NORTH-HOLLAND PUBLISHING COMPANY

# POSITRONFIT: A VERSATILE PROGRAM FOR ANALYSING POSITRON LIFETIME SPECTRA

Peter KIRKEGAARD
*Reactor Physics Department, Danish Atomic Energy Commission Research Establishment Risö*
*DK-4000 Roskilde, Denmark*

and

Morten ELDRUP
*Chemistry Department, Danish Atomic Energy Commission Research Establishment Risö,*
*DK-4000 Roskilde, Denmark*

Received 16 November 1971

## PROGRAM SUMMARY

*Title of program*: POSITRONFIT

*Catalogue number*: AAGK

*Computer*: B6700, *Installation*: Risö, Denmark;
IBM 360/75*. NEUCC, Denmark

*Operating system or monitor under which the program is executed*: B6700 MCP Mark II.00

*Programming language used*: FORTRAN

*High speed store required*: 20000 words. *No. of bits in a word*: 48

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1125

*Keywords*: Atomic, Nuclear, Positron, Lifetime, Time Spectrum, Source Correction, Least Squares, Fitting, Convolution, Minimization, Sum-of-exponentials, Iterations, Marquardt, Constraints, Covariance Matrix.

*Nature of the physical problem*

In a condensed material positrons may annihilate at several different characteristic rates. A measured positron lifetime spectrum will therefore consist of a sum of decaying exponential functions with different decay rates, smeared somewhat owing to the finite time resolution of the measuring system and superimposed on a constant background.

*Method of solution*

Positron lifetime spectra are analysed by an iterative least-squares technique of the semi-linear Marquardt [1] type. The mathematical model is a sum of decaying exponentials convoluted with a gaussian resolution function, and with a constant background added. Fixed values can be imposed on any number of lifetimes and relative intensities. Correction for the source annihilation is taken into account. A statistical analysis is made resulting in the covariance matrix of the estimated parameters

*Restrictions on the complexity of the program*

The program in its present version is restricted to include up to four lifetime components. The maximum number of channels in the multichannel analyser is 512, and of these max. 400 are used in the analysis.

*Reference*

[1] D. W. Marquardt, J. Soc. Ind. Appl. Math. 11 (1963) 431.

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* With minor changes.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 256–268. NORTH-HOLLAND PUBLISHING COMPANY

# FINE STRUCTURE CROSS SECTIONS FROM REACTANCE MATRICES

H. E. SARAPH

*Physics Department, University College, London W.C.1, UK*

Received 8 November 1971

## PROGRAM SUMMARY

*Title of program*: JAJOM

*Catalogue number*: AAGJ

*Computer*: IBM 360/65. *Installation*: Computer Centre, University College London

*Operating system*: OS/360

*Programming language used*: FORTRAN IV

*High speed storage required*: 40844 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer; Card Punch

*No. of cards in combined program and test deck*: 2109

*Keywords*: Atomic, Scattering, Inelastic, Cross Section, Reactance Matrix, Russell Saunders Coupling, *J J* Coupling, Fine Structure Transitions, Energy Level, Collision Strength, Racah Coefficient.

*Nature of the physical problem*

The reactance matrices obtained from calculations in *SL* coupling are transformed to compute collision strengths for transitions between fine structure levels.

*Method of solution*

The data which follow the same conventions as described in ref. [1] are sorted and checked. The *R*-matrices are transformed to pair coupling using algebraic recoupling coefficients. Moreover, the *R*-matrices may be transformed to allow for intermediate coupling in the target if the required transformation coefficients are available. The collision strengths are computed from the *R*-matrices using matrix algebra.

*Restrictions on the complexity of the problem*

The array lengths should be adjusted to suit the user's problem and the core available on his computer. The algebraic transformations may introduce numerical inaccuracies for angular momenta $> 15$, if single precision is used.

*Typical running time*

The sample data, comprising one energy, 6 target terms with summation over 20 intermediate states, took 2 minutes.

*Unusual features of the program*

On the 360/65, use of double precision is recommended. Instructions are given for conversion to single precision. Elaborate checks are made by the program at all stages of the computations and detailed error messages are printed. Use of the MACRO processor [2] is recommended. The SCOPE CHECKPOINT/RESTART can easily be introduced, a suitable spot is marked in MAIN by a comment card.

*References*

[1] H. E. Saraph, Computer Phys. Commun. 1 (1970) 232.
[2] A. C. Day, Technical Report 2, Computer Centre, University College London (1971).

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 269–271. NORTH-HOLLAND PUBLISHING COMAPNY

# PROGRAM ACQN TO CALCULATE TRANSPORT COLLISION INTEGRALS ADAPTED TO RUN ON IBM COMPUTERS

P. D. NEUFELD and R. A. AZIZ

*Department of Physics, The University of Waterloo, Waterloo, Ontario, Canada*

Received 22 November 1971

## ADAPTATION SUMMARY

*Title of adaptation*: ACQN ADAPTED FOR IBM 360/75

*Adaptation number*: 0001

*Reference to original program*:

*Catalogue number*: ACQN; *Title*: TRANSPORT COLLISION INTEGRALS; *Ref. in CPC*: 2 (1971) 47.

*Authors of original program*: H. O'Hara and F. J. Smith

*Computer*: IBM 360/75. *Installation*: University of Waterloo

*Operating system*: OS/360

*Programming language used in adapted program*: IBM FORTRAN IV

*High speed store required*: 23500 words. *No. of bits in a word*: 32

*No. of cards required to effect adaptation (including directive cards)*: 412

*Typical running time*

On the IBM 360/75 using FORTRAN H and a machine language object deck to eliminate compile time, the test run is executed in 18 seconds.

*Reference*

[1] H. O'Hara and F. J. Smith, Computer Phys. Commun. 2 (1971) 47.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 275–276. NORTH-HOLLAND PUBLISHING COMPANY

# ERRATUM NOTICES

*Title of manuscript*: Distorted wave Born approximation for direct reactions

*Authors*: T. Tamura, W.R. Coker and F. Rybicki

*Reference*: Computer Physics Communications 2 (1971) 94.

*Title of program*: DWBA–VENUS

*Catalogue number*: ABOH

*Title of manuscript:* Coulomb functions for complex energies
*Authors:* T. Tamura and F. Rybicki
*Reference:* Computer Physics Communications 1 (1969) 25.
*Title of program:* COULOM
*Catalogue number:* ABOC

C-142

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 318–321. NORTH-HOLLAND PUBLISHING COMPANY

# THE REDUCED ROTATION MATRIX *

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*Princeton University, New Jersey 08540, USA*

and

J.G. CRAMER
*University of Washington, Seattle, Washington 98105, USA*

Received 8 March 1972

## PROGRAM SUMMARY

*Title of program:* DS

*Catalogue number:* ABOR

*Computer*: IBM 360/91. *Installation*: Princeton University

*Operating system*: OS360

*Programming languages used*: FORTRAN IV

*High speed store required:* 947 words. *No of bits in a word:* 64

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck:* 112

*Keywords*: Atomic, Molecular, Nuclear, Rotation Matrix, Rotation Group, Representation, Euler Angle, Symmetry, Helicity, Correlation.

*Nature of the physical problem*

Subprogram DS is a FORTRAN IV DOUBLE PRECISION FUNCTION which calculates the reduced matrix elements of finite rotations [1] in the angular momentum representation, using a standard phase convention [2]. The four arguments of the FUNCTION are: J2, twice the total angular momentum; MI2 and MF2, twice the $z$-projection of the total angular momentum in the initial and final coordinate systems, respectively and BETA, the Euler angle-of-rotation around $y'$ [2].

*Method of solution*

A Wigner-closed-sum expression for $d^j_{mm'}(\beta)$ is evaluated. Each term contains products of factorials. Using a method similar to that of Wills [3], a common coefficient (containing factorials) is evaluated by combining the logarithms of the factorials, followed by one exponentiation. The remaining expression is written, without factorials, as a nested product. This method contrasts well, in speed and accuracy, with methods that evaluate factorial products in the closed-sum coefficients term-by-term, before adding.

*References*

[1] E.P. Wigner, Gruppentheorie (vieweg, Braunschweig, 1931); A.R. Edmonds, Angular momentum in quantum mechanics (Princeton Univ. Press, Princeton, 1960).
[2] D.M. Brink and G.R. Satchler, Angular momentum (Oxford Univ. Press, London, 1962).
[3] J.G. Wills, Oak Ridge National Laboratory Report ORNL-TM-1949 (1967), unpublished; Computer Phys. Commun. 2 (1971) 381.

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* Supported in part by the US Atomic Energy Commission.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 322–333. NORTH-HOLLAND PUBLISHING COMPANY

# THE COMPUTATION OF THE GROWTH OF A GASEOUS DISCHARGE IN SPACE-CHARGE DISTORTED FIELDS

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*Singleton Park, Swansea SA2 8PP, UK*

Received 8 March 1972

## PROGRAM SUMMARY

*Title of program*: SPARK71

*Catalogue number*: ABUD

*Computer*: ICL 1905E. *Installation:* Computer Centre, University College of Swansea,
ICL ATLAS. Atlas Computer Laboratory Chilton, Didcot, U.K.

*Operating system*: GEORGE 2

*Programming language used*: FORTRAN

*High speed storage required*: 18600 words. *No. of bits in a word*: 32

*Is the program overlaid* ? No

*No. of magnetic tapes required*: 2 at most

*What other peripherals are used* ? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1075

*Keywords*: Plasma, Atomic, Electrical Discharge, Electrical Breakdown, Space-charge, Plane-parallel Electrodes, Positive Ion, Electron, Photon, Cathode.

*Nature of physical problem*

SPARK71 computes the growth of ionization currents flowing between parallel plane electrodes. The effects which are incorporated are primary ionization, secondary cathode emission due to the incidence of photons and ions, space-charge distortion of the applied field, and the properties of the external electrical circuit.

*Method of solution*

The hyperbolic differential equations describing the growth of ionization in one dimension are integrated along the two characteristic directions in the $x$–$t$ plane [1,2]. Iteration in the $t$ direction allows the change in the coefficients of the equations (due to field distortion) to be followed. The electric field is found from an approximation to the correct three-dimensional distribution [3]. The $x$ axis is divided into equal-length meshes, and the time step is chosen to minimise the number of iterations needed.

*Restrictions on the complexity of the problem*

As given in the listing, the program will accommodate up to 80 meshes in the $x$ direction, and up to 4 photon secondary processes, each with its own characteristic delay time. (These numbers may be increased by changing the DIMENSION statements only.)

*References*

[1] A.J. Davies, C.J. Evans and F. Llewellyn Jones, Proc. Roy. Soc. A281 (1965) 164.
[2] A.J. Davies, C.S. Davies and C.J. Evans, Proc. IEE 118 (1971) 816.
[3] A.J. Davies and C.J. Evans, Proc. IEE 114 (1967) 1547.

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 334–338. NORTH-HOLLAND PUBLISHING COMPANY

# NUMERICAL SOLUTION OF THE RADIAL SCHRÖDINGER EQUATION

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*MTA, Müszaki Fizikai Kutató Intézete, Budapest, IV. Fóti-ut 56 (Pf. 76), Hungary*

Received 25 May 1971
Revised manuscript received 24 March 1972

## PROGRAM SUMMARY

*Title of program*: SCHROD

*Catalogue number*: ACQZ

*Computer*: CDC-3300. *Installation:* Computing Centre of the Hungarian Academy of Sciences

*Operating system*: MASTER

*Programming languages used*: USASI FORTRAN

*High speed store required*: 9500 words. No. of bits in word: 24

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Printer

*No. of cards in combined program and test deck*: 138

*Keywords*: Atomic, Solid State, Schrödinger Equation, Potential, Scattering, Runge–Kutta, Band Structure, Muffin-tin.

*Nature of physical problem*

The subroutine SCHR solves the radial Schrödinger equation using a logarithmic mesh without transforming the independent variable. It is applicable in problems where a smooth expansion of the scale near the origin is advantageous.

*Method of solution*

Given the potential, the starting and the final value of the independent variable and the number of mesh points, the program calculates a suitable logarithmic mesh and integrates the radial Schrödinger equation using a special Runge–Kutta method. It is written as a subroutine with emphasis on its applicability in "muffin-tin" type band structure calculations.

*Restictions on the complexity of the problem*

For a given energy the subroutine solves the Schrödinger equation for the angular momentum values $l_{\mathrm{min}} \leqslant l \leqslant l_{\mathrm{max}}$.

*Typical running time*

Compile time is a few seconds, the execution time depends on the number of mesh used-roughly (number of mesh points) × (25 multiplication/division times + 15 addition times) × (number of different $l$ values).

COMPUTER PHYSICS COMMUNICATIONS 3 (1972) 339–350. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTER SIMULATION OF MÖSSBAUER SCATTERING SPECTRA *

J. L. GROVES

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Received 11 October 1971
Revised manuscript received 28 January 1972

## PROGRAM SUMMARY

*Title of program*: MÖSSBAUER SCATTERING SPECTRA

*Catalogue number*: ABOP

*Computer*: IBM 360/75. *Installation*: University of Illinois

*Operating system*: HASP – OS/MVT

*Programming language used*: FORTRAN IV

*High speed storage required*: 81K words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer; Card Punch

*No. of cards in combined program and test deck*: 1942

*Keywords*: Nuclear, Solid State, Mössbauer Effect, Scattering Spectrum, Computer Simulation.

*Nature of physical problem*

We have written a FORTRAN computer program for simulating Mössbauer scattering spectra for large scatterers and large detectors.

*Method of solution*

We calculate the intensities and energies of the allowed transitions and form the scattering spectrum as a function of the angles locating the scatterer and detector. We then numerically integrate the spectrum over the solid angles subtended by the scatterer and detector.

*Restrictions on the complexity of the problem*

The simulated spectra are restricted to an axially symmetric source-scatterer-detector arrangement, and the hamiltonian describing the hyperfine interactions of the Mössbauer nuclei with external fields must be diagonal in the $|IM\rangle$ representation.

*Typical running time*

A typical CPU time for a 512 channel, 18-line spectrum using the IBM 360/75 computer is 2 seconds.

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* Work supported by the National Science Foundation under grant NSF GP 17135.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 107–116. NORTH-HOLLAND PUBLISHING COMPANY

# A MULTI-CONFIGURATION HARTREE–FOCK PROGRAM WITH IMPROVED STABILITY

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*Department of Applied Analysis and Computer Science,*
*Faculty of Mathematics, University of Waterloo, Waterloo, Ontario, Canada*

Received 19 April 1972

## PROGRAM SUMMARY

*Title of program:* MCHF72

*Catalogue number:* ACRF

*Computer:* IBM S360/75. *Installation:* University of Waterloo, Waterloo, Ontario, Canada

*Operating system:* OS/360-MVT and HASP II

*Programming languages used:* FORTRAN IV

*High speed store required:* 53k words. *No. of bits in a word:* 32

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* Card Reader; Punch; Printer

*No. of cards in combined program and test deck:* 2780

*Reference to other published version of this program:*
*Catalogue number:* ACQJ; *Title:* MULTI-CONFIGURATION HARTREE–FOCK; Ref. in CPC: 1 (1969) 151

*Keywords:* Atomic Structure, Numerical Hartree–Fock, Configuration Interaction, Bound State, Schrödinger Equation, Wavefunction, Self-Consistent Field, Energy Level.

*Nature of physical problem*

Numerical non-relativistic Hartree–Fock results are determined within the multi-configuration approximation for atoms in a bound state.

*Method of solution*

The self-consistent field method of solution is employed. In a multi-configuration calculation the mixing coefficients are adjusted periodically as part of the SCF iteration. Two new methods are used for the solution of the differential equarions [1]. Otherwise the program is essentially the same as MULTI-CONFIGURATION HARTREE–FOCK [2] but with improved accuracy and efficiency.

The orthogonality conditions

$$\int P(nl;r)\,P(n'l;r)\,\mathrm{d}r = \delta_{nn'},$$

may be applied to either functions within a configuration or else all functions. These conditions lead to off-diagonal energy parameters in the Hartree–Fock equations.

*Restrictions on the complexity of the problem*

The possible configurations are restricted to those for which the interactions can be expressed as either $F^k$, $G^k$, or $R^k$ integrals. This excludes certain singly substituted configurations which frequently would result in an indeterminate system of equations [3]. Also, since bound states in the continuum interact most strongly with continuum states, a multi-configuration calculation for such states cannot be performed with this program.

*Unusual features of the program*

The organization of the program is such that the "frozen core" approximation may be used and orbitals with zero occupation number are allowed.

*Typical running time*

The CPU time for a series of cases consisting of

(i) the two-configuration approximation for $C^{2+}$, $B^+$ and Be $^1S$

(ii) Na 3p $^2P$

(iii) Na 3s $^2S$ with 1s, 2s, 2p "frozen"

(iv) Na 4s $^2S$ with 1s, 2s, 2p "frozen" and the 3s having a zero occupation number

required 1.06 min on an IBM 360/75.

*References*

[1] C. Froese Fischer, J. Comp. Phys. 10 (1972), to be published.

[2] C. Froese Fischer, Computer Phys. Commun. 1 (1969) 151.

[3] C. Froese Fischer, J. Phys. B. 3 (1970) 779.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 117–127. NORTH-HOLLAND PUBLISHING COMPANY

# RECURSIVE NUMERICAL INTEGRATION OF MULTI-PARTICLE PHASE SPACE WITH PERIPHERAL MATRIX ELEMENT

P. PIRALÄ * and E. BYCKLING **

*University of Helsinki, Research Institute for Theoretical Physics, 00170 Helsinki 17, Finland*

Received 17 January 1972

## PROGRAM SUMMARY

*Title of program*: PERIPHERAL PHASE SPACE INTEGRAL

*Catalogue number*: AAUD

*Computer*: UNIVAC 1108, *Installation*: SITRA, Helsinki, Finland

*Operating system*: EXEC 8

*Programming languages used*: FORTRAN IV

*High speed store required*: 21097 words. *No. of bits in a word*: 36

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer.

*No. of cards in combined program and test deck*: 860

*Keywords*: Nuclear, High Energy, Particle Physics, Phase Space Integral, Peripheral, Recursive Integration, Cross Section.

*Nature of physical problem*

The program calculates the total cross section of a multiparticle final state as a function of total energy, when the matrix element is of the form $\exp(a_1t_1+a_2t_2+...+a_{n-1}t_{n-1})$. This cross section is proportional to the volume of "peripheral phase space".

*Method of solution*

The program is based on a recursive integration formula [1]. At each recursion step the same integrand is integrated over many different integration areas, which are two-dimensional and bounded by a hyperbola and a straight line. The two-dimensional integrals are calculated by a method based on Simpson's formula.

*Restrictions on the complexity of the problem*

Multiplicity of the final state between 3 and 20.

*Typical running time*

2 min for about 5 per cent accuracy, multiplicities 3–8 and 100 energy values.

*Reference*

[1] E. Byckling and K. Kajantie, Phys. Rev. 187 (1969) 2008.

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* Present address: CERN, Geneva, Switzerland.

** On leave of absence from University of Jyväskylä.

COMPUTER PHYSICS COMMUNICATION 4 (1972) 128–137. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR COMPUTING LEVEL CROSSINGS AND THE BACK–GOUDSMIT EFFECT

Paolo VIOLINO

*Gruppo Nazionale Struttura della Materia, Istituto di Fisica dell' Università, Pisa, Italy*

Received 25 January 1972

## PROGRAM SUMMARY

*Title of program*: BACK–GOUDSMIT

*Catalogue number*: ACRD

*Computer*: IBM 360/67, *Installation* CNUCE – Pisa

*Operating system*: OS or CMS

*Programming languages used*: FORTRAN IV

*High speed store required*: 7176 Words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer; Card Punch

*No. of cards in combined program and test deck*: 400

*Keywords*: Atomic, Zeeman Effect, Back–Goudsmit Effect, Paschen–Back Effect, Hyperfine Structure, Fine Structure, Level-Crossings, Radiofrequency Transitions.

*Nature of physical problem*

Several techniques of atomic spectroscopy, like hfs measurements, level crossings, Hanle effect (when the hfs is of the order of the width of a level), all require a precise knowledge of the positions of the sublevels of a fine or hyperfine multiplet as functions of the applied magnetic field. When the quantum numbers $I$ and $J$ (or $S$ and $L$, according to the representation which is being used) are larger than ½, this requires the solution of the secular equation. This is carried out by this computer program, which can compute as well the positions of the level crossings between specified levels.

*Method of solution*

The description of the secular equation to be solved is given in ref. [1]. The solution is carried out by computing the secular matrix from the input data and then diagonalizing it. The positions of the level crossings are computed by an iterative procedure.

*Restrictions on the complexity of the problem*

The program is designed to handle quantum numbers $I$ and $J$ (or $S$ and $L$) whose sum does not exceed 7. It can be easily extended to higher values by changing a few FORMAT statements.

*Typical running time*

Compilation time is about 9 sec, assembling and loading time is about 1 sec, and execution time of the test run is about 4 sec, on the 360/67 computer of the CNUCE.

*Unusual features of the program*

The program contains a few diagnostic features that alert the user whenever his requirements are not compatible with the physical nature of the problem. Owing to its short computation time, the program can easily be used to evaluate the $A$ and $B$ hfs couping constants from an experimental set of level-crossing positions by an interpolation method [2].

*References*

[1] J. Kapelewski and K. Rosiński, Acta Phys. Polon. 28 (1965) 177.

[2] D. Schönberner and D. Zimmermann, Z. Physik 216 (1968) 172.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 138–146. NORTH-HOLLAND PUBLISHING COMPANY

# THE TWO-NUCLEON EFFECTIVE-RANGE PARAMETERS WITH TENSOR FORCES

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*Istituto di Fisica dell'Università di Pisa, Pisa, Italy*
*and Istituto di Fisica Nucleare, Sezione di Pisa, Pisa, Italy*

Received 22 March 1972

## PROGRAM SUMMARY

*Title of program:* EFFECTIVE RANGE APPROXIMATION

*Catalogue number:* ABGJ

*Computer:* IBM 7090. *Installation:* Pisa University, Pisa, Italy.

*Operating system or monitor under which the program is executed:* IBSYS Version 13 (IBJOB Processor Version 5)

*Programming language used:* FORTRAN IV

*High speed storage required:* 23000 words. *No. of bits in a word:* 36

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* None

*No. of cards in combined program and test deck:* 385

*CPC Library subprograms used:*
*Catalogue number:* ABGE; *Title:* DEUT; Ref in CPC: 2 (1971) 353
*Adaption number:* 0001; *Title:* REMOVE NON-STANDARD FORTRAN; Ref in CPC: 4 (1972) 140

*Keywords:* Nuclear, Two-Nucleon, Neutron–Proton, Schrödinger Equation, Tensor Forces, Wavefunctions, Zero Energy Scattering, Scattering Length, Effective Range.

*Nature of physical problem*

Subroutine EFRNG is a FORTRAN IV subroutine designed to calculate the zero energy wavefunction of the neutron–proton $J=1^+$ state when the interaction between the particles is described by a given combination of central, tensor and spin–orbit potentials with or without a hard core. From this one derives the effective range parameters, viz. the scattering length and effective range in terms of which can be expressed the low energy scattering behaviour. This subroutine may also be employed in the research of phenomenological potentials where a rapid and accurate calculation is required.

*Method of solution*

The problem is similar to that of obtaining the bound state solution of the two-nucleon Schrödinger equation in the presence of tensor forces presented in ref. [1], and several of the subroutines which formed part of the program DEUT (catalogue number: ABGE) are used by the present program.

The method of calculation employed follows closely the treatment presented in ref. [2]. The technique used involves a direct numerical integration of the differential equations; the requirement that the wavefunctions vanish at the origin, that they behave asymptotically in an analytically well-determined way together with the employment of middle point matching determines the wavefunctions of the zero energy state uniquely.

*Restrictions on the complexity of the problem*

The interparticle potentials considered in the program are those used in ref. [1], namely, the Hamada–Johnston potential [3] and the Reid hard-core or soft-core potentials [4]. To use EFRNG (or DEUT) in the case of some other potential one must simply re-write the subprogram POT.

*Typical running time*

The test case requires 65 seconds to compile and 6 seconds to run on the IBM 7090 computer at Pisa University.

*References*

[1] L. Lovitch and S. Rosati, Computer Phys. Commun. 2 (1971) 353.
[2] L. Lovitch and S. Rosati, Proc. Phys. Soc. (London) 88 (1966) 909.
[3] T. Hamada and I.D. Johnston, Nucl. Phys. 34 (1962) 382.
[4] R.V. Reid, Ann. Phys. 50 (1968) 411.

## ADAPTION SUMMARY

*Title of adaption:* REMOVE NON-STANDARD FORTRAN

*Adaption number:* 0001

*Reference to original program:*
*Catalogue number:* ABGE; *Title:* DEUT; Ref in CPC: 2 (1971) 353

*Authors of original program:* L. Lovitch and S. Rosati

*Computer:* IBM 7090; IBM 360/67. *Installation:* Pisa University

*No. of cards required to effect adaption (including directive cards):* 138

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 221–226. NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAMS FOR COMPUTING THE LOGARITHM OF THE GAMMA FUNCTION, AND THE DIGAMMA FUNCTION, FOR COMPLEX ARGUMENT

K.S. KÖLBIG
*CERN, Geneva, Switzerland*

Received 10 May 1972

## PROGRAM SUMMARY

*Title of program*: CLOGAM AND CDIGAM

*Catalogue number*: ACRG

*Computer*: CDC 6600, *Installation*: CERN, Geneva

*Operating system*: CDC scope

*Programming languages used*: FORTRAN IV

*High speed store required*: 334 (CLOGAM), 232 (CDIGAM) words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Line Printer

*No. of cards in combined program and test deck*: 161

*Keywords*: General Purpose, Nuclear, Atomic, Gamma Function, Logarithm of Gamma Function, Psi Function, Digamma Function, Asymptotic Expansion, Coulomb, Phase Shift, Scattering, Schrödinger

*Nature of the physical problem*

The gamma function $\Gamma(z)$, its logarithm $\ln \Gamma(z)$, and its logarithmic derivative $\psi(z) = \mathrm{d} \ln \Gamma(z)/\mathrm{d}z$ appear in a wide range of physical applications. We mention here only the Veneziano model and its generalizations in high-energy physics, and the Coulomb phase shift for complex energies.

*Method of solution*

For $\operatorname{Re} z \geqslant 7$, the asymptotic expansions are used to compute $\ln \Gamma(z)$ and $\psi(\bar{z})$. For other regions of the $z$ plane, suitable functional relations are used. Care is taken that $\operatorname{Im} \ln \Gamma(z)$ is computed correctly, and not merely modulo $2\pi$.

*Restrictions on the complexity on the problem*

As the tests show, an accuracy of 12–14 significant digits is normally obtained.

*Running time*

Typical running times (in microseconds on the CDC 6600) are given in table 1.

Table 1

| | $\ln \Gamma(z)$ (CLOGAM) | $\psi(z)$ (CDIGAM) |
|---|---|---|
| $\operatorname{Re} z < -6$ | 580 | 570 |
| $-6 \leqslant \operatorname{Re} z < 0$ | 790 | 650 |
| $0 \leqslant \operatorname{Re} z < 7$ | 630 | 390 |
| $7 \leqslant \operatorname{Re} z$ | 330 | 300 |

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 227–232. NORTH-HOLLAND PUBLISHING COMPANY

# RELATIVISTIC KINEMATICS FOR TWO-BODY FINAL STATES *

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*and University of Washington, Seattle, Washington 98105, USA*

Received 30 March 1972

## PROGRAM SUMMARY

*Title of program*: TWOBDY

*Catalogue number*: ABOS

*Computer*: IBM 360/91. *Installation*: Princeton University

*Operating system*: OS 360

*Programming language used*: FORTRAN IV

*High speed store required*: 1597 words. *No. of bits in a word*: 64

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 185

*Keywords*: Nuclear, Collision, Reaction, Kinematics, Two-Body, Relativistic, Final States, Conservation, Symmetry.

*Nature of the physical problem*

Although two-body reactions occur within a plane, it is convenient to specify all momentum vectors using three-dimensional rectangular coordinates. Such a formulation [1, 2] permits different orientations of the beam or that of the detected outgoing particles to be more easily described. Use of rectangular coordinates to describe both position and momentum is convenient for finite-geometry kinematic calculations and results in greater speed of calculation since trancendental functions, (other than square root) are avoided.

*Method of solution*

All particle types are assumed known (this specifies each rest mass). Since the reaction $Q$-value is deemed convenient for input, it has been used to calculate the rest mass of the second outgoing particle. The direction of emission ($\hat{P}_1$) of outgoing particle 1 is taken as input, leaving four unknowns: $P_1$ and $P_2$. Conservation of 4-momentum ($P_0$, $E_0$) yields a set of 4 equations which are solved by FORTRAN IV subroutine TWOBDY, providing the needed information. This subroutine additionally provides the jacobian of the transformation from laboratory to centre-of-mass frame (i.e., $\delta \Omega_L / \delta \Omega_C$). TWOBDY is lengthened by this inclusion, so users not needing centre-of-mass information are referred to subroutine TWOBOD in program BODY3 [3] which is considerably shorter. This jacobian is used in the "test program" to provide a value for kinematic broadening (i.e., $\delta E_1 / \delta \theta_1$). The "test

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* Supported in part by the National Science Foundation and the U.S. Atomic Energy Commission.

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program" generates a table of kinematic values for both the laboratory and centre-of-mass by enumerating, in equal step sizes, the in-plane laboratory-angle-of-emission of one outgoing particle (called PART.3). The program enumerates its laboratory energy, its corresponding centre-of-mass angle, its transformation jacobian ($\delta\Omega_L/\delta\Omega_C$), its kinematic broadening ($\delta E/\delta\theta$), as well as the laboratory energy and angle of the second (recoil) particle. The output format is nearly the same as that of HEEWEE [4]. Both kinematic branches are treated when appropriate.

*References*

[1] W.J. Braithwaite, Ph.D. thesis, University of Washington (1971), unpublished.
[2] W.J. Braithwaite, Nucl. Phys. Lab. Ann. Rept., Univ. of Washington (1971), unpublished.
[3] W.J. Braithwaite, Computer Phys. Commun. 4 (1972) 233.
[4] D.L. Hendrie and R.W. West, stored in the repository HOARD, Nucl. Phys. Lab., Univ. of Washington, Seattle, Washington.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 233–238. NORTH-HOLLAND PUBLISHING COMPANY

# RELATIVISTIC KINEMATICS FOR THREE-BODY FINAL STATES *

W.J. BRAITHWAITE**

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*and University of Washington, Seattle, Washington 98105, USA*

Received 30 March 1972

## PROGRAM SUMMARY

*Title of program*: BODY3

*Catalogue number*: ABOT

*Computer*: IBM 360/91. *Installation*: Princeton University

*Operating system*: OS 360

*Programming languages used*: FORTRAN IV

*High speed store required*: 1166 words. *No. of bits in a word*: 64

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 128

*Keywords*: Nuclear, Collision, Reaction, Kinematics, Three-body, Relativistic, Final States, Conservation, Symmetry.

*Nature of the physical problem*

Kinematically complete relativistic reaction kinematics are calculated for 3-body final states using the principle of conservation of momentum-energy ($P_0$, $E_0$) (i.e., 4-momentum conservation) for an isolated system. This program takes, as input, the rest masses of all the particles (except that of the target), the reaction $Q$-value, the 3-momentum of outgoing particle 1 ($P_1$) and the emission direction of outgoing particle 2 ($\hat{P}_2$). The three-body kinematics problem is then reduced to an equivalent 2-body kinematics problem by constructing effective total momentum–energy values for the subsystem of outgoing particles 2 and 3 (i.e., $P_{\text{eff}} = P_0 - P_1$ and $E_{\text{eff}} = E_0 - E_1$) [1].

*Method of solution*

The equivalent 2-body kinematics problem is solved using the FORTRAN IV subroutine TWOBOD. This subroutine is particularly convenient to use as it describes the input momenta and the (unnormalized) direction of particle 2 in terms of their rectangular components in any arbitrarily oriented cartesian 3-space. Following the output style [2] of a previously written program [3], the "test program" generates a table of kinematic values by enumerating, in equal step sizes, the kinetic energy of outgoing particle 1. This table gives the laboratory kinetic energy of outgoing particles 2 and 3, the relative energy of each particle pair ($E_{23}$, $E_{12}$, $E_{13}$), and the outgoing direction ($\theta$, $\varphi$) of particle 3. Both kinematic branches are included, when applicable.

*References*

[1] W.J. Braithwaite, Ph.D. thesis, Univ. of Washington (1971) p. 73, unpublished.

[2] J.G. Cramer, private communication.

[3] W.J. Braithwaite and J.G. Cramer, Nucl. Phys. Lab. Ann. Rept., Univ. of Washington (1970) p. 46, unpublished.

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* Supported in part by the U.S. Atomic Energy Commission.

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COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 239–248. NORTH-HOLLAND PUBLISHING COMPANY

# A NUCLEAR HARTREE–FOCK INTRINSIC WAVEFUNCTION PROJECTION PROGRAM

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M. HADJ HASSAN and M. LAMBERT
*Institut de Physique Nucléaire, Villeurbanne (69), France*

Received 18 November 1971

## PROGRAM SUMMARY

*Title of program*: PROJ

*Catalogue number*: ABGI

*Computer*: IBM 360/40. *Installation*: Institut Mécanographique, Algiers, Algeria

*Operating system*: DOS

*Programming languages used*: FORTRAN IV

*High speed store required*: 19 K words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 1094

*Keywords*: Nuclear, Schrödinger Equation, Rotational Band, Peierls–Yoccoz Method.

*Nature of physical problem*

PROJ calculates energies of the rotational band generated by a nuclear wavefunction $\Phi_M$ which is an eigenstate of $J_z$ with the eigenvalue $M$. $\Phi_M$ may be obtained by using program HARFOCK [1]. The two-body interaction must be a sum of two gaussian potentials with arbitrary spin, isospin and space-exchange terms.

*Method of solution*

The energy of each rotational state is evaluated by the Peierls–Yoccoz formula [2,3]. For each value of the rotation angle, $\beta$, chosen by the integration program, the matrix elements occurring are evaluated.

*Restrictions on the complexity of the problem*

The geometrical basis includes the 1s, 1p and 2s, 1d deformed shells. The program works with 40 occupied and unoccupied orbitals. The interaction must be exponential. The c.m. two-body elements are taken into account but the Coulomb interaction is neglected. Orbitals must be eigenstates of $J_z$ and $\tau_z$. $M$ must be positive or equal to 0.

*References*

[1] J.F. Allard, A. Abzouzi and B. Houssais, Comp. Phys. Commun. 3 (1972) 22.
[2] R.E. Peierls and J. Yoccoz, Proc. Phys. Soc. A 70 (1957) 381.
[3] J. Yoccoz, Proc. Phys. Soc. A 70 (1957) 388.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 249–256. NORTH-HOLLAND PUBLISHING COMPANY

# EXTERNAL MODES OF MOLECULAR CRYSTALS

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Received 4 April 1972

## ADAPTATION SUMMARY

*Title of Adaptation*: EXTERNAL MODES

*Adaptation number*: 0001

*Reference to original program*:

*Catalogue number*: ACMI; *Title*: GROUP THEORY OF LATTICE DYNAMICS, Ref. in CPC: 3 (1972) 88.

*Authors of original program*: T.G. Worlton and J.L. Warren

*No. of cards required to effect adaption (including directive cards)*: 158

*Additional keywords*: Molecular Vibrations, Normal Modes, External Modes.

*Nature of physical problem*

This adaptation modifies "GROUP THEORY OF LATTICE DYNAMICS" [1] to calculate the symmetry properties of the external modes of vibration of molecular crystals [2].

*Restrictions on the complexity of the problem*

Solutions are given in terms of the cartesian axes. Redundant coordinates for linear molecules are not eliminated.

*Typical running time*

20 seconds.

*References*

[1] T.G. Worlton and J.L. Warren, Computer Phys. Commun. 3 (1972) 88.
[2] G. Venkataraman and V.C. Sahni, Rev. Mod. Phys. 42 (1970) 409.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 257–261. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR NORMALISED MORSE FUNCTIONS

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*Department of Mathematics, Polytechnic of North London, London N7 8DB, UK*

Received 4 May 1972

## PROGRAM SUMMARY

*Title of program*: MORSEFNS

*Catalogue number*: AAGM

*Computer*: ICL 1905E. *Installation*: LPCU, Polytechnic of N. London

*Operating system*: GEORGE 2

*Programming language used*: FORTRAN

*High speed storage required*: 2K words. *No. of bits in a word*: 48

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer (for test only)

*No. of cards in combined program and test deck*: 136

*CPC Library subprograms used*: None

*Reference to other published version of this program*: None

*Keywords*: Molecular Physics, Morse Functions, Eigenfunctions, Schrödinger Equation, Bound States.

*Nature of physical problem*

To produce the normalised eigenfunctions of the Schrödinger equation with the Morse potential [1].

*Method of solution*

The subroutine calculates the solution obtained by Morse, correctly normalised, by evaluating the polynomial solution at a set of given points.

*Restrictions on the complexity of the program*

It is assumed that the parameters given to the subroutine are constants typical of problems involving real molecules.

*Typical running time*

On the ICL 1905E the test program takes 13s mill time. In general the execution time depends on the number of points at which the results are required.

*Reference*

[1] P.M. Morse, Phys. Rev. 34 (1929) 57.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 262–267. NORTH-HOLLAND PUBLISHING COMPANY

# ENERGY LEVEL CALCULATIONS WITH AROVMI MODEL *

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*Universidad de Buenos Aires, Pabellón No. 2, Ciudad Universitaria, Buenos Aires, Argentina*

## PROGRAM SUMMARY

*Title of program*: AROVMI

*Catalogue number*: ABMC

*Computer*: IBM 360/50. *Installation*: Centro de Computación, Facultad de Ingeniería, UBA, Buenos Aires, Argentina

*Operating system*: OS/360

*Programming languages used*: FORTRAN IV

*High speed store required*: 28000 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 493

*CPC Library subprogram used:*
*Catalogue number*: ABOE; *Title*: ENERGY LEVELS IN DAVYDOV MODEL; Ref. in CPC: 2 (1971) 33.

*Keywords*: Nuclear, Energy Level, Energy Ratio, AROVMI Model, Davydov–Filippov Model, Bessel Interpolation Formula, Newton–Raphson Method, Double Linear Interpolation, Root Mean Square Overall Deviation.

*Nature of physical problem*

This program provides the theoretical values for the energy levels and ratios calculated with the AROVMI model [1] in terms of the parameters $\gamma$ and $\rho$.

*Method of solution*

A combination of graphical and numerical procedures is used to find the actual values of the model parameters. The Bessel formula is applied to interpolate energy levels predicted by the Davydov–Filippov model [2]. The Newton–Raphson method is employed to find the root of a cubic equation.

*Restrictions on the complexity of the problem*

This program can be used for nuclei having combinations of experimental energy ratios $R(^14)$ and $R(^22)$ which fall within the bounds depicted in fig. 1a and b in the long write-up. Computations are performed with the energy levels of the ground-state rotational band from $I = 2$ up to 20 (by steps of 2) and those of the anomalous (gamma) band for $I = 2$ up to 10 (by steps of 1).

*References*

[1] S.M. Abecasis and E.S. Hernández, Nucl. Phys. A180 (1972) 485.
[2] A.S. Davydov and G.F. Filippov, Nucl. Phys. 8 (1958) 237.

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* Work done under the partial auspices of the Consejo Nacional de Investigaciones Científicas y Técnicas, Argentina.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 268–274. NORTH-HOLLAND PUBLISHING COMPANY

# VECTOR COUPLING COEFFICIENTS AS PRODUCTS OF PRIME FACTORS

R.McD. DODDS and G. WIECHERS *
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Received 28 February 1972
Revised manuscript received 23 May 1972

## PROGRAM SUMMARY

*Title of program*: COEF

*Catalogue number*: ACRE

*Computer*: ICL 1901A, *Installation*: University of Port Elizabeth

*Operating system*: ICL automatic operator

*Programming languages used*: FORTRAN IV

*High speed store required*: 14080 words. *No. of bits in a word*: 24

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 625

*Keywords*: Atomic Physics, Nuclear Physics, Vector Coupling Coefficient, Spectroscopy, Rotation Matrix, Clebsch–Gordan Coefficient, Racah Coefficient, Integer Arithmetic.

*Nature of physical problem*

The program computes 3*j*-symbols, 6*j*-symbols and rotation matrices (special case) and expresses the result as a product of powers of prime numbers.

*Method of solution*

A set of subroutines is given to generate prime numbers, to express a given integer as a product of prime numbers and to carry out addition, subtraction, multiplication and division of such products, always leaving the result in the form of a product of prime numbers.

*Typical running time*

The time depends on the magnitude of the arguments of the coefficients, and is between 2 and 10 seconds. Running time is greatly reduced after the first few coefficients have been calculated.

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COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 347–360. NORTH-HOLLAND PUBLISHING COMPANY

# GEOMAGNETIC FIELD MODELS: SCALAR AND VECTOR POTENTIAL, INDUCTION VECTOR AND ITS GRADIENT TENSOR COMPUTED BY A COMMON ALGORITHM

G. KLUGE
*ESOC, 6100 Darmstadt, Germany*

Received 11 May 1972

## PROGRAM SUMMARY

*Title of program*: MAGNES

*Catalogue number*: AAEC

*Computer*: IBM 360/65. *Installation*: ESOC, Darmstadt

*Operating system*: 360 - OS

*Programming language used*: FORTRAN IV

*High speed storage required*: 833 words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* None

*No. of cards in combined program and test deck*: 206

*CPC Library subprograms used*: Catalogue number: AAEA; title: SHELL; ref. in CPC: 3(1972) 31

*Keywords*: Geophysics, Space Science, Geomagnetic Field, Potential Theory, Harmonic Polynomials, Spherical Harmonics, Stokes' Theorem, Vector Potential, Inverse Radii.

*Nature of physical problem*

The program has been written for handling phenomenological models of the geomagnetic field; it can be adapted to any spherical harmonic expansion of potentials (e.g. gravitational or electrostatic).

*Method of solution*

The scalar potential is expressed as a harmonic polynomial in terms of Cartesian coordinates with reciprocal radius. Derivatives of any order can be simply calculated in a way similar to Horner's procedure. This results in a unified algorithm for the various field quantities and also facilitates the generation and use of local approximations to field models.

*Typical running time*

For a field model of degree 8 (i.e. 80 coefficients): 3 msec for the scalar and vector potential, additional 3 msec for the induction vector, further 3 msec for the gradient tensor.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 361–370. NORTH-HOLLAND PUBLISHING COMPANY

# SYMMETRIZED PROGRAM FOR CALCULATING ENERGY BANDS AND ELECTRONIC STRUCTURE OF SOLIDS

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and

M. BELAKHOVSKY
*Centre d'Etudes Nucléaires de Grenoble, 38 043 Grenoble CEDEX, France*

Received 29 June 1972

## PROGRAM SUMMARY

*Title of program*: SYMMETRIZED APW

*Catalogue number*: ACMJ

*Computer*: IBM 360/67. *Installation*: Institut de Mathématiques Appliqués, 38 - Grenoble, France

*Operating system*: OS 360/67

*Programming language used*: FORTRAN IV

*High speed storage required*: 108864 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 2124

*Keywords*: Solid State, Band Structure, Symmetrized Augmented Plane Wave Method.

*Nature of the physical problem*

The program calculates the energy bands and electronic structure of solids. It is written to include two different atoms per unit cell.

*Method of solution*

The method of calculation is the augmented plane wave method with the point group symmetry of the hamiltonian taken into account. The program includes subroutines dealing with the symmetry part of the band structure which have been described earlier [1, 2]. For simplicity and completeness they are repeated, slightly modified, in this deck.

*Restrictions on the complexity of the problem*

Limited to cubic lattices.

*Typical running time*

9 seconds per point for a 3 by 3 SAPW matrix.

*References*

[1] V. Hoffstein and O. Moller, Computer Phys. Commun. 2 (1971) 17.
[2] V. Hoffstein and O. Moller, Computer Phys. Commun. 2 (1971) 26.

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[*] Laboratoire associé au Centre Nationale de la Recherche Scientifique (C.N.R.S.).

COMPUTER PHYSICS COMMUNICATIONS 4(1972) 371–376. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTATION OF CROSS SECTIONS AND POLARIZATIONS FOR NUCLEAR REACTIONS, IN WHICH ONLY SPIN 1/2 PARTICLES ARE INVOLVED

P. HEISS
*Institut für Theoretische Physik der Universität zu Köln, Köln, Germany*

Received 12 September 1972

## PROGRAM SUMMARY

*Title of program*: S 1/2 PARTICLE CS AND POL

*Catalogue number*: ABGK

*Computer*: IBM 370/165. *Installation*: KFA Jülich

*Operating system*: OS

*Programming language used*: FORTRAN IV

*High speed storage required*: 10302 words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 356

*Keywords*: Nuclear Reactions, *S*-matrix, *M*-matrix, Cross Sections, Polarization, Phase Shifts.

*Nature of physical problem*

Both for a phase shift analysis [1] and for reaction calculations [2] one needs to relate cross sections, polarization values, etc. on the one hand and *S*-matrix elements in the ususal *lsJ* representation on the other. For general cases this calculation requires great computational effort [3]. For reactions in which only spin $\frac{1}{2}$ particles are involved this effort can be considerably reduced, by the explicit calculation of the *M*-matrix [4].

*Method of solution*

In the special case under discussion, relatively simple relations between *S*-matrix elements and *M*-matrix elements can be derived [4]. From *M*-matrix elements, cross sections and polarizations can be obtained in a simple way. Hence, the following program requires only a small amount of high speed storage space and runs relatively fast.

*Restrictions*

The program is restricted to a maximum angular momentum of $L = 3$. If higher partial waves are included, dimensions of certain arrays have to be increased. These arrays are specified in section 3 of the “long write-up”.

*Typical running time*

Half a second per energy value.

*References*

[1] R. Kankowsky and D. Fick, Computer Phys. Commun. 2 (1971) 223.
[2] P. Heiss and H.H. Hackenbroich, Nucl. Phys. A182 (1972) 522.
[3] R.D. McCulloch et al., ORNL Report 4121.
[4] T.A. Tombrello, C.M. Jones, G.C. Phillips and J.L. Weil, Nucl. Phys. 39 (1962) 541.

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 377–381. NORTH-HOLLAND PUBLISHING COMPANY

# CFPJJ–FRACTIONAL PARENTAGE COEFFICIENTS FOR EQUIVALENT ELECTRONS IN *jj*-COUPLING

I.P. GRANT

*Mathematical Institute, University of Oxford, Oxford, UK*

Received 20 September 1972

## PROGRAM SUMMARY

*Title of program:* CFPJJ – CFP IN JJ-COUPLING

*Catalogue number:* ACRI

*Computer*: ICL 1906A. *Installation*: Oxford University, UK
IBM 370/165 CECAM, Batiment 506, 91–Campus d'Orsay, France

*Operating system*: GEORGE 3, Mark 6.3

*Programming language used*: FORTRAN IV (XFIV compiler)

*High speed store*: 3941. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and testdeck*: 441

*Keywords*: Atomic, *jj*-coupling, Coefficients of Fractional Parentage.

*Nature of physical problem*

Antisymmetric wavefunctions of $N$ identical particles can be expressed as linear combinations of antisymmetric wavefunctions for $(N-1)$ such particles multiplied by single-particle wavefunctions with the aid of coefficients of fractional parentage [1–3]. When the particles are electrons described by Dirac's equation, it is natural to use *jj*-coupling, so that the coefficients denoted by

$$(j^N(v, w, J)\,\{|j^{N-1}(\bar{v}, \bar{w}, \bar{J})\,, j)$$

are required, the state on the left being referred to as the "daughter", and that with barred quantum numbers on the right being a "parent". Here $j$ is the total angular momentum of a single electron, and $j^N(v, w, J)$ denotes a state of $N \leqslant 2j+1$ such electrons whose total angular momentum quantum number is $J$, seniority $v$, whilst $w$ is any other quantum number needed to resolve any further degeneracy [2]. These coefficients are needed, for example, in the MCP package [4] for evaluating angular momentum coefficients in relativistic atomic structure calculations involving open shells.

*Method of solution*

A tabular search using the tables given in refs. [2] and [5] is used. The data is stored in integer form to avoid difficulties arising from word lengths in going from one machine to another.

*Restrictions on complexity of the problem*

All coefficients with $j = \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$ are tabulated. Attempts to find a coefficient for $j = \frac{1}{2}$ or for $j \geqslant \frac{9}{2}$ with $n \geqslant 2$ will cause termination of the run.

*References*

[1] G. Racah, Phys. Rev. 63 (1943) 367.
[2] A.R. Edmonds and B.H. Flowers, Proc. Roy. Soc. A214 (1952) 515.
[3] J.C. Slater, Quantum theory of atomic structure, Vol. 2 (McGraw-Hill, New York, 1960).
[4] I.P. Grant, Computer Phys. Commun., to be published.
[5] A. de-Shalit and I. Talmi, Nuclear shell theory (Academic Press, New York, 1963).

COMPUTER PHYSICS COMMUNICATIONS 4 (1972) 382–383. NORTH-HOLLAND PUBLISHING COMPANY

# ERRATUM

T.G. Worlton and J.L. Warren, Group-theoretical analysis of lattice vibrations, Computer Physics Communications 3 (1972) 88–117.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 56–63. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR CLOSED ORBIT MINIMIZATION BY ANALYTIC TECHNIQUE

J.V. TROTMAN

*Nimrod, Accelerator and Beams Theory Group, Rutherford High Energy Laboratory,*
*Chilton, Didcot, Berkshire, UK*

Received 12 May 1972

## PROGRAM SUMMARY

*Title of program:* COMBAT

*Catalogue number:* ABCF

*Computer:* IBM 360/195 IBM 360/175 *Installation:* R.H.E.L. IBM 360/195 Chilton, Didcot, Berkshire, UK

*Operating system:* OS (IBM 360)

*Programming language used:* FORTRAN 4

*High speed store required:* 40K words. *No. of bits in a word:* 32

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck:* 1036

*Keywords:* Nuclear, High Energy, General, Closed Orbit, Minimization, Synchrotron.

*Nature of physical problem*

Closed orbit errors resulting from guide field imperfections in a sychrotron, increase the magnet aperture required. It is impractical to eliminate all imperfections but it is possible to minimise the closed errors by a suitable arrangement of correcting elements and beam sensors. For minimisation one must calculate the correlation between the distorted closed orbit and the correcting elements.

*Method of solution*

The correlation between the distorted closed orbit and the correcting elements may be expressed as a set of linear simultaneous equations:

$$\boldsymbol{c} = [A]\ [\mathrm{C}]^{-1} y,$$

$\boldsymbol{c}$ = necessary correction, $\boldsymbol{y}$ = closed orbit distortion vector. The matrix $[A]$ is tri-diagonal, the coefficients being functions of the $(2 \times 2)$ linear transfer matrices of the machine components. The matrix $[C]$ is bi-diagonal with leading diagonal terms equal to unity. $[\mathrm{C}]^{-1}$ is readily obtained algebraically. In general the sub-diagonal terms are much less than unity and $[\mathrm{C}]^{-1}$ may therefore be considered a correcting matrix. The solution of the matrix equation may be obtained to any order of accuracy desired: from the full analytic solution to the zeroth order approximation. The zeroth order approximation considers the matrix $[\mathrm{C}]^{-1} \equiv [I]$. For the *n*th order approximation only *n*th order products are retained in $[\mathrm{C}]^{-1}$.

*Unusual features*

Previous mathematical techniques involved inversion or eigenvalue analysis of large matrices. COMBAT determines the correlation coefficients by evaluation of simple algebraic expressions. The storage required by COMBAT is comparatively small and execution is rapid.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 64–68. NORTH-HOLLAND PUBLISHING COMPANY

# AN EXPANSION EQUATION OF STATE SUBROUTINE

K. MORGAN*
*UKAEA, AWRE, Aldermaston, Berkshire, UK*

Received 1 September 1972

## PROGRAM SUMMARY

*Title of program:* EOSEXP

*Catalogue number:* ACSA

*Computer:* ICL ATLAS 2, *Installation:* UKAEA, AWRE, Aldermaston

*Operating system:* ATLAS Supervisor

*Programming language used*: FORTRAN

*High speed storage required:* 2600 words. *No. of bits in a word:* 48

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* Card Reader; Printer

*No. of cards in combined program and test deck:* 424

*Keywords:* Fluid Dynamics, Equation of State, Change of State.

*Nature of the physical problem*

Hydrodynamic calculations of physical systems require suitable equations of state for the materials of interest. EOSEXP is an expansion equation of state subroutine which can be used to give a realistic description of the single-phase and two-phase behaviour of an expanding material, provided that conditions along the saturation curve for this material can be tabulated.

*Method of solution*

In the single-phase region a Grüneisen type equation of state is used to obtain the pressure given the specific internal energy and the specific volume. In the two-phase region an implicit equation is solved for the temperature, and the pressure is then obtained by using the relationship between pressure and temperature valid along the saturation curve.

*Typical running time*

On the AWRE ATLAS loading and compilation of the test deck takes 17 sec. The running time depends on the number of times the equation of state subroutine is entered. Typically the calculation of 10 state points (5 single-phase and 5 two-phase) requires a CPU time of 4 sec.

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COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 69–79. NORTH-HOLLAND PUBLISHING COMPANY

# A NUCLEAR OPTICAL MODEL CODE FOR SMALL COMPUTERS

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*Physics Department, University of North Carolina, Chapel Hill, North Carolina 27514, USA,*
*and Triangle Universities Nuclear Laboratory, Durham, North Carolina 27706, USA*

and

R.A. HARDEKOPF ‡
*Physics Department, Duke University and Triangle Universities Nuclear Laboratory,*
*Durham, North Carolina 27706, USA*

Received 7 August 1972

*Title of Program*: OPTICS

*Catalogue number*: ABOU

| *Computer*: | *Installation:* |
|---|---|
| Honeywell DDP 224 | Triangle Universities Nuclear Laboratory |
| IBM 370/165 | Triangle Universities Computation Center |
| Xerox Data System XDS 930 | Los Alamos Scientific Laboratory |

*Operating system:* DDP: None, IBM: HASP Version 3.0, Release 20.6, XDS: Local

*Programming Language:* Fortran IV

*High speed core required*: DDP: 8K words; *No. of bits in a word:* 24, with 2 words per single precision floating-point variable, 1 word per single precision integer variable.
IBM: 80K bytes: *No. of bits in a byte*: 8, with 4 bytes per single precision floating point variable, 4 or 2 bytes per single precision integer variable.
XDS: 6.2K words: *No. of bits in a word*: 24, with 2 words per extended precision floating-point variable, 1 word per single precision integer variable.

*Is the program overlaid?* DDP: Yes, IBM: No, XDS: Yes

*No. of magnetic tapes required*: DDP: 1, IBM: none, XDS: none

*What other peripherals used*: DDP: Card Reader, Line Printer, Typewriter, Oscilloscope Display
IBM: Card Reader, Line Printer
XDS: Card Reader, Line Printer, Typewriter, Oscilloscope Display, Magnetic Drum

*No. of cards in combined program and test deck*: 3344

*Keywords*: Nuclear, Optical Model, Potential, Elastic Scattering, Schrödinger Equation, Spin-zero, Spin-half, Spin-one, Spin–orbit, Fox–Goodwin, Coulomb, Compound-elastic, Scattering Amplitudes, Phase Shifts, Transmission Coefficients, Angular Distributions, Cross Sections, Vector Polarization Analysing Power, Tensor Polarization Analysing Power.

*Nature of physical problem*

OPTICS performs non-relativistic calculations of differential cross sections and vector and tensor polarization analysing powers for the elastic scattering of a particle of spin $s = 0, \frac{1}{2}$ or 1 from a particle whose spin is ignored. Scattering data are analysed in terms of an optical model potential including spin orbit coupling (for $s = \frac{1}{2}, 1$) and an optional compound-elastic cross-section calculation.

‡ Present address: Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87544, USA.

### *Method of solution*

Coulomb wavefunctions are generated [1] at two points exterior to the nuclear potential. Nuclear scattering wavefunctions are produced by outward iteration of the Schrödinger equation using method VII of Fox and Goodwin [2] (also known as the Cowell and Noumerov methods [3]). Matching of these wavefunctions at the two points produces scattering amplitudes which are used to generate differential cross sections and polarization components and, if necessary, the transmission coefficients for the compound-elastic cross-section calculation [4].

### *Restrictions on the complexity of the problem*

Maximum projectile spin is 1; target spin is ignored. The only spin dependent potential is spin orbit. The maximum number of $L$-values is 30. The maximum number of radial mesh points is 200. The maximum number of experimental differential cross section points is 32. The maximum number of experimental differential polarization points is 32 (only one polarization component at a time for $s = 1$). No program-controlled search facility.

### *Typical running time*

For a single shot calculation without compound-elastic and exclusive of input/output, calculation time is

$$\text{Time} \approx T_\text{c}(2S+1)\, M_\text{T}^{\frac{1}{3}}(M_\text{p}E)^{\frac{1}{2}} \times 10^{-2}\ \text{sec}\,,$$

where $T_\text{c}$ is computer multiply time in μsec, $S$ is spin, $M_\text{T}$ is target mass, $M_\text{p}$ is projectile mass, $E$ is laboratory energy.

### *Unusual features*

This program fits into a small computer, permitting both batch-processing and interactive data analysis. The oscilloscope display allows simultaneous comparison of up to 3 calculated angular distributions with the data. A compound-elastic calculation is included. Scattering amplitudes or phase shifts can be input to produce angular distributions.

### *References*

[1] B. Buck, R.N. Maddison and P.E. Hodgson, Phil. Mag. 5 (1960) 1181.

[2] L. Fox and E.T. Goodwin, Proc. Cambridge Phil. Soc. 45 (1949) 373.

[3] M.A. Melkanoff, T. Sawada and J. Raynal, in: Methods in computational physics, Vol. 6 (1966) 1.

[4] P.A. Moldauer, Phys. Rev. 135 (1964), B642, section IV.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 80–87. NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAM FOR EVALUATION OF NON-EXCHANGE TYPE INTEGRALS REQUIRED IN ELECTRON-ATOM SCATTERING THEORY USING SLATER-TYPE ORBITALS AS BASIS FUNCTIONS*

Richard L. SMITH and Donald G. TRUHLAR
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*Minneapolis, Minnesota 55455, USA*

Received 11 August 1972

## PROGRAM SUMMARY

*Title of program:* NETI

*Catalogue number:* AAGP

*Computer:* CDC 6600; *Installation:* University Computer Center of the University of Minnesota

*Operating system:* SCOPE

*Programming language used:* FORTRAN IV

*High speed storage required:* 9900 words. *No. of bits in a word:* 60

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* Card reader; Line printer

*No. of cards in combined program and test deck:* 1100

*Reference to other published version of this program:* Catalogue number: AAGT; Title: NETIX, Ref. in CPC: 5 (1973) 81

*Keywords:* Atomic, Integrals, Continuum Wavefunctions, Electron–Atom Scattering, Variational Method, Spherical Bessel Functions, Numerical Quadrature, Summation of Series, Born Approximation, Scattering Amplitude, X-ray Form Factor, Scattering Factor, Two-center Coulomb Integrals.

*Nature of the physical problem*

The problem of electron scattering from atoms and other quantum mechanical scattering problems can be solved using algebraic variational methods [1]. This program computes the five basic integrals in terms of which all the nonexchange-type integrals which are needed for the scattering calculation can be expressed.

*Method of solution*

The integrals are evaluated using the procedures of Lyons and Nesbet [2, 3]. We believe these procedures are the fastest methods which can be used to obtain the desired accuracy. In some cases alternative subroutines are provided which use the methods suggested by Bottcher [4].

*Restrictions on the complexity of the problem*

We use the notation of Lyons and Nesbet [2] in the following. For the method used, the parameters $\lambda$, $\mu$, $p$, and $q$ must be non-negative integers, the real parts of $\alpha$ and $\beta$ must be non-negative, and $k_1$ and $k_2$ must be non-negative and real. Also in our programs, $\alpha$, $\beta$ must be real except in the $G$ integral.

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* Research supported in part by the National Science Foundation under research grant no. GP-28684 and by the Graduate School of the University of Minnesota.

*Typical running times*

Typical running times (CPU time) per integral for machine accuracy are: $G$, 0.0005 sec; $H$, 0.07 sec; $I$, 0.02 sec; $V$, 0.3 sec; and $W$, 0.005 sec. These times are strong functions of the particular parameter values for each integral. The test run requires 6 sec (excluding compilation and loading).

*Unusual features of the program*

Parameters are included in the program which will allow a user to try different methods of solutions or different accuracy for the $G$ and/or $I$ integrals to achieve a faster possible running time for a given accuracy for a given problem.

*References*

[1] F.E. Harris and H.H. Michels, Methods Comp. Phys. 10 (1971) 144.
[2] J.D. Lyons and R.K. Nesbet, J. Comp. Phys. 4 (1969) 499.
[3] J.D. Lyons and R.K. Nesbet, J. Comp. Phys., to be published.
[4] C. Bottcher, J. Comp. Phys. 6 (1970) 237.

## PROGRAM SUMMARY

*Title of program:* NETIX

*Catalogue number:* AAGT

*Computer:* CDC 6600; *Installation:* University Computer Center of the University of Minnesota

*Operating system:* SCOPE

*Programming language used:* FORTRAN IV

*High speed storage required:* 13800 words. *No. of bits in a word:* 60

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* None

*No. of cards in combined program and test deck:* 1319

*Reference to other published version of this program:* Catalogue number: AAGP; Title: NETI; Ref. in CPC: 5 (1973) 80

*Keywords:* Atomic, Integrals, Continuum Wavefunctions, Electron–Atom Scattering, Variational Method, Spherical Bessel Functions, Numerical Quadrature, Summation of Series, Born approximation, Scattering Amplitude, X-ray Form Factor, Scattering Factor, Two-center Coulomb Integrals.

*Nature of physical problem*

This is the double precision version of NETI.

*Typical running time*

Typical running times (CPU time) per integral for machine accuracy are: $G$, 0.002 sec; $H$, 0.3 sec; $I$, 0.08 sec; $V$, 1 sec; and $W$, 0.02 sec. These times are strong functions of the particular parameter values for each integral. The test run requires 26 sec (excluding compilation and loading).

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COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 153–160. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTATION OF EFFECTIVE REGGE TRAJECTORIES FOR HIGH ENERGY TWO-BODY REACTIONS*

D.J. HARRISON, A.C. IRVING and A.D. MARTIN
*Department of Physics, University of Durham, UK*

Received 12 May 1972

## PROGRAM SUMMARY

*Title of program:* EFFECTIVE REGGE TRAJECTORIES

*Catalogue number:* ABCE

*Computer:* IBM 360/67; *Installation:* Northumbrian Universities Multiple Access Computer, Durham, UK

*Operating system or monitor under which the program is executed:* MICHIGAN TERMINAL SYSTEM

*Programming language used:* FORTRAN IV

*High speed storage required:* 46K words. *No. of bits in a word:* 32

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck:* 1381

*Keywords:* Nuclear, High Energy, Particle, Differential Cross Section, Slope, Normalisation, Effective Regge Trajectory, Chew–Frautschi Plot, Least-squares.

*Nature of physical problem*

Regge theory forms the basis of most of the current attempts to understand the strong interactions of elementary particles. Consequently as a preliminary to any serious analysis of high-energy data for two-body reactions it is desirable to extract the effective Regge trajectory from the differential cross section ($d\sigma/dt$) data for each reaction under study. A program has therefore been written to calculate these effective trajectories from the data. The program includes the option of determining the $t$-independent overall normalization of a given experiment, and it calculates the slope of the differential cross section, and the integrated cross section.

*Method of solution*

The effective Regge trajectory, $\alpha_{\text{eff}}(t)$, for a given $t$ is determined by first interpolating the experimental $d\sigma/dt$ to obtain values at the same $t$- but different $s$-values (where $s$ is the square of the c.m. energy and $-t$ is the square of the 4-momentum transfer). The $\alpha_{\text{eff}}$ is then calculated by performing a least-squares fit of $\ln(d\sigma/dt)$ to $\ln s$. Several $t$-values are fitted simultaneously so that the normalization of an experiment at a given $s$-value may be determined. Further, for a given energy, $\ln(d\sigma/dt)$ can be parametrised by a polynomial in $t$ of degree specified by the user, and a least-squares fit is used to calculate the parameters from the experimental data.

*Restrictions on the complexity of the problem*

A maximum of six different reactions may be analysed in one run. For each reaction $d\sigma/dt$ data can be used at up to 20 different momenta, and $\alpha_{\text{eff}}$ can be calculated at up to 20 different $t$-values.

*Typical running time*

About eight seconds to calculate $\alpha_{\text{eff}}$ at six $t$-values using $d\sigma/dt$ data at eight different momenta.

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* Work supported by the Science Research Council.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 163–215. NORTH-HOLLAND PUBLISHING COMPANY

# USERS MANUAL FOR THE OPTIME SYSTEM*

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*Berkeley, California 94720, USA*

Received 9 February 1972
Revised manuscript received 30 May 1972

## PROGRAM SUMMARY

*Title of program:* OPTIME SYSTEM

*Catalogue number:* AAYB

*Computer:* CDC 6600, *Installation:* Lawrence Berkeley Laboratory, Berkeley, California

*Operating system:* BKY

*Programming languages used:* FORTRAN, 6000 Compass

*High speed storage required:* 32K–60K words. *No. of bits in a word:* 60

*Is the program overlaid?* No.

*No. of magnetic tapes required:* Minimum 0, Maximum 6

*What other peripherals are used?* Card Reader; Line Printer; Disc in lieu of Tape Files.

*No. of cards in combined program and test deck:* 10992

*Keywords:* General Purpose, Nuclear, High Energy, Fitting, Maximum Likelihood, Least Squares, Maximization, Estimator, Likelihood function, Chisquare Function, Expectation Value, Reference Function, Gram-Schmidt Orthonormalization, Error Matrix, Histogram, Monte Carlo Event Generation, Preferred Frequency Distribution.

*Nature of physical problem*

The OPTIME System [1] is an assembly of subroutines for fitting theoretical expressions to statistical distributions, especially those arising in particle physics. The system also provides for calculating error matrices, performing integrations, and making histograms.

*Method of solution*

The program adjusts parameters of the theoretical expression by using various estimators and maximization techniques combined with special stepping procedures, some of which use approximations for the second derivative matrix. The quality of the fit should be judged by analysis of the printout, inspection of the error matrix, and inspection of histograms of the data with the fitted curve superposed.

*Restrictions on the complexity of the problem*

This program is usable for functions with any number of variable parameters subject only to available core space and running time. The user function of parameters $|a|$ and variable $|x|$ (whose value is either the data point $|\xi|_k$ or the integration point $|x|_l$) must be proportional to the expectation value of the distribution of data points at $|x|$ for the true values of $|a|$. When integration points in the fit have weights $\Omega_l, \Sigma\, \Omega_l y(|x|_l, |a|)$ must approximate the integral of $y$. If the Monte Carlo event generator in the OPTIME System is used, $\Omega_l$ reconstitutes phase space, and the function $y(|x|, |a|)$ corresponds to the square of the matrix element.

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* Work done under auspices of the U.S. Atomic Energy Commission

*Typical running time*

The typical running time for fitting a function of three linear variable parameters, using 500 experimental data points and 3000 Monte Carlo integration points, with convergence in one step, is about 76 seconds of CP-time on a CDC-6600. This includes 46 seconds of CP-time to compile the complete program.

*Unusual features of the program*

The program allows for experimental data points to be weighted, for example, to allow for detection efficiencies in particle physics.

Since the standard OPTIME System allocates blank COMMON dynamically during execution, only a minimal amount of blank COMMON is declared initially. Once the variable parameters and buffer sizes are specified, the necessary blank COMMON is allocated by a call to a SUBROUTINE OPTIME which adjusts the field length. This is feasible on the CDC machine because blank COMMON is located at the high end of the user's block of core. To disable this scheme check in the subroutines IMME, RAME, STORME, and COCHIS how much blank COMMON is required in each case, declare the maximum amount initially in the main program, and replace the standard SUBROUTINE OPTIME by

```
SUBROUTINE OPTIME
RETURN
END
```

or eliminate the calls to this subroutine.

*Reference*

[1] P.H. Eberhard and W.O. Koellner, Computer Phys. Commun. 3 (1972) 396.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 217–224. NORTH-HOLLAND PUBLISHING COMPANY

# APPROXIMATION FORMULA AND ALGOL PROGRAM OF THE LORENTZ-INVARIANT MOMENTUM-SPACE INTEGRAL FOR PARTICLES OF EQUAL MASSES

Arthur JABS
*Universität Trier–Kaiserslautern, Fachbereich Physik, Kaiserslautern, Germany*

Received 17 January 1972

## PROGRAM SUMMARY

*Title of program*: LIMS

*Catalogue number*: AAUE

*Computer*: Univac 1108. *Installation*: University of Karlsruhe, remote station University Kaiserslautern

*Operating system*: EXEC 8

*Programming language used*: ALGOL 60

*High speed storage required*: 5951 words; *No. of bits in a word*: 36

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 187

*Keywords*: Nuclear, High Energy, Multi-Particle Production, Phase Space, Momentum Space, Statistical Model.

*Nature of the physical problem*

In high-energy particle reactions the transition probability can be written as the product of some squared transition-matrix element and the volume of momentum space of the outgoing particles. The statistical hypothesis means putting this matrix element independent of the individual particles' momenta, so that the transition probability is proportional to some momentum space integral. This idea, with due modifications, has proved rather useful in describing particle production spectra [1] and in providing a well defined "kinematical" background from which can be distinguished "dynamical" effects such as resonances. The special case of equal masses gains interest from the fact that mostly pions are produced, and that the colliding nucleons are excluded from the statistical ensemble because they carry away a large fraction of their initial energy. Moreover, the special case can advantageously be used in comparisons between Lorentz-invariant and non-invariant momentum space [2] as well as in studies of the high-particle-number limit.

*Method of solution*

The evaluation is based on the work of Lurçat and Mazur [3]. Restriction on the special case of equal masses has made it possible to approximate the formulae of [3] by relatively simple expressions. In addition, a correction factor has been introduced which reduces the relative error to less than 0.5% for any values of the variables.

*References*

[1] R. Hagedorn, Nuovo Cimento 56A (1968) 1027; Nucl. Phys. B24 (1970) 93, and references therein; J.R. Wayland and T. Bowen, Nuovo Cimento 48A (1967) 663; G. Zgrablich and J.R. Wayland, Phys. Rev. D1 (1970) 1501, and references therein; A. Jabs, Z. Phys. 222 (1969) 1.

[2] A. Jabs, Nucl. Phys. B34 (1971) 177.

[3] F. Lurçat and P. Mazur, Nuovo Cimento 31 (1964) 140.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 225–238. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTER SIMULATIONS OF MÖSSBAUER SPECTRA FOR AN EFFECTIVE SPIN $S = \frac{1}{2}$ HAMILTONIAN[‡]

E. MÜNCK, J.L. GROVES, T.A. TUMOLILLO[‡‡] and P.G. DEBRUNNER
*Department of Physics, University of Illinois, Urbana, Illinois 61801, USA*

Received 26 June 1972

## PROGRAM SUMMARY

*Title of program*: PARAMAGNETIC MÖSSBAUER SPECTRA

*Catalogue number*: ABMD

*Computer*: IBM 360/75. *Installation*: University of Illinois

*Operating system*: HASP-OS/MVT

*Programming language used*: FORTRAN IV

*High speed storage required*: 35 K words. *No. of bits in a word*: 64

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer; Card Punch.

*No. of cards in combined program and test deck*: 1698

*Keywords*: Nuclear, Solid State, Mössbauer Spectra, Spin 1/2 Hamiltonian, Iron-57, Polycrystalline Sample.

*Nature of physical problem*

We have written a computer program that calculates the Mössbauer spectra of $^{57}$Fe in paramagnetic polycrystalline samples in an external magnetic field, $H$, using a spin hamiltonian of the form

$$\mathcal{H} = \beta_e \boldsymbol{S} \cdot \mathbf{g} \cdot \boldsymbol{H} + \boldsymbol{S} \cdot \mathsf{A} \cdot \boldsymbol{I} + \boldsymbol{I} \cdot \mathsf{P} \cdot \boldsymbol{I} - g_n \beta_n \boldsymbol{H} \cdot \boldsymbol{I}.$$

Here $\mathbf{g}$, $\mathsf{A}$, and $\mathsf{P}$ are tensors describing the electronic Zeeman interaction, the magnetic hyperfine interaction and the quadrupole interaction, respectively. The tensors $\mathbf{g}$, $\mathsf{A}$, and $\mathsf{P}$ are allowed to have different principal axes systems.

*Method of solution*

An expression for the intensity of a Mössbauer spectrum is derived. The expression contains Clebsch–Gordan coefficients, functions describing the absorption of radiation as a function of the angle between the observation direction and the nuclear quantization axis, a line-shape function, and coefficients which describe the nuclear eigenstates as linear combinations of the eigenstates of the nuclear spin operators. The coefficients are obtained by solving the spin hamiltonian.

*Restrictions on the complexity of the problem*

The external field, $H$, is assumed to be sufficiently large ($H \gg 20$ G) to make the electronic Zeeman term much greater than any other term in the hamiltonian. The electron spin relaxation time is long compared to the nuclear precession time. The spin doublet described by the hamiltonian must be sufficiently isolated from other electronic states such that the applied field $H$ does not mix other levels into the spin doublet. In practice this condition is fulfilled for fields less than 1 kG.

*Typical running time*

A typical CPU time for a 256 channel spectrum calculated with 18 × 18 integrations over $\beta_0$ and $\gamma_0$ is 25 sec.

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[‡] Work supported in part by grants from the National Science Foundation, NSF GP 26282, and U.S. Public Health Service GM 16406.

[‡‡] Present address: Department of Physics, Kansas State University, Manhattan, Kansas 66502, USA.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 239–262. NORTH-HOLLAND PUBLISHING COMPANY

# ELECTRON ENERGY DEPOSITION IN A GASEOUS MIXTURE

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*Department of Physics and Astronomy, University of Florida, Gainsville, Florida 32601, U.S.A.*

Received 13 April 1972
Revised manuscript received 20 September 1972

## PROGRAM SUMMARY

*Title of program*: ELECTRON ENERGY LOSS

*Catalogue number*: ACRH

*Computer*: IBM 360/65. *Installation*: University of Florida Computing Center

*Operating system*: SYSTEM/360

*Programming language used*: FORTRAN IV

*High speed store required*: 36864 words. No. of bits in a word: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*What other peripherals are used?* Card Reader; Line Printer

*No. of cards in combined program and test deck*: 2223

*Keywords descriptive of problem and method of solution*: Atomic, Astrophysics, Molecular, Electron Impact, Scattering, Excitation, Ionization, Energy Degradation, Loss Function, Continuous Slowdown Approximation, Aurora, Airglow, Radiation.

*Nature of physical problem*

This program apportions the energy deposited in various atomic and molecular excitations and ionizations when an electron impinges upon a prescribed mixture of gases. The basic electron impact cross sections for each species are inserted using parameterized forms which have been found to adequately represent such data. Relative populations and excitation efficiencies for all atomic or molecular states are computed following the complete energy degradation of the primary electron and all generations of secondaries formed during ionization events.

*Method of solution*

The method of solution has evolved in a series of works [1–3]. In this formulation, the continuous slowdown approximation is assumed along with the condition of local absorption of the electron beam. The loss function $L(E) = -(1/n)\,\mathrm{d}E/\mathrm{d}x$ plays the central role. It can be constructed internally from the complete sets of input cross sections or it can be estimated externally and read into the program along with the relevant subset of cross sections. The energy bookkeeping calculations then reduce to numerical or analytical integration of functions involving cross sections and the loss function.

*Restrictions on the complexity of the problem*

Standardized parameterized forms must be used for inserting cross sections. These are available for a number of important atmospheric gases. However, many options are available which make the program very flexible.

*Typical running time*

The running time is variable depending upon detailed input. Runs involving one gas with a total of 5 ionization continua and ≈ 20 excitation states require about 15 seconds when the electron is degraded from 1 keV.

*References*

[1] A.E.S. Green and C.A. Barth, J. Geophys. Res. 70 (1965) 1083.
[2] R.S. Stolarski and A.E.S. Green, J. Geophys. Res. 72 (1967) 3967.
[3] L.R. Peterson and A.E.S. Green, J. Phys. B (Proc. Phys. Soc.) 1 (1968) 1131.

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† Present address: Aerodyne Research, Inc., Burlington, Massachusetts 01803, USA

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 263–282. NORTH-HOLLAND PUBLISHING COMPANY

# A GENERAL PROGRAM TO CALCULATE ANGULAR MOMENTUM COEFFICIENTS IN RELATIVISTIC ATOMIC STRUCTURE

I.P. GRANT
*Mathematical Institute, University of Oxford, Oxford, UK*

Received 16 October 1972

## PROGRAM SUMMARY

*Title of program*: MCP

*Catalogue number*: ACRJ

*Computer*: ICL 1906A, *Installation*: Oxford University, Oxford, UK;
IBM 370/165, CECAM, Batiment 506, 91-Campus d'Orsay, France

*Operating system*: GEORGE 3, Mark 6.3

*Programming language used*: FORTRAN IV (XFIV compiler)

*High speed storage required*: 32K words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card Reader; Line Printer

*No. of cards in combined program and test deck*: 2317

*CPC Library subprograms used*:

| *Catalogue number* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAGD | NJSYM | 1 (1970) 241, 2 (1971) 173 |
| AAGD0002 | ADAPT TO INTEGER ARITHMETIC | 5 (1973) 161 |
| ACRI | CFPJJ–CFP IN JJ-COUPLING | 4 (1972) 377 |

*Keywords*: Atomic, Configuration Interaction, Racah, Coefficients of Fractional Parentage, Recoupling Coefficients, Slater Integrals, Complex Atoms, Relativistic, Dirac Equation, Wavefunction, Bound States, *jj*-coupling.

*Nature of physical problem*

A number of relativistic atomic structure programs have recently become available, for example the self-consistent field programs of Liberman et al. [1] and Desclaux et al. [2]. This makes it possible to consider carrying out configuration interaction calculations using Dirac wavefunctions. As in the non-relativistic theory, the major difficulty is to determine the two-electron matrix elements of the interelectronic interaction. This program calculates the coefficients of Slater integrals in terms of which the matrix elements can be expressed.

*Method of solution*

The coefficients of Slater integrals can be derived by combining the standard expressions of the relativistic formulation [3] with the schemes of Fano [4] or Armstrong [5]. As in the equivalent non-relativistic program of Hibbert [6], the coefficients can be expressed as a sum of terms incorporating products of fractional parentage coefficients [7], recoupling coefficients [8] and reduced matrix elements.

Configurations are defined by the number of electrons in each occupied shell, the (*nja*) quantum numbers and angular momentum couplings.

*Restrictions on the complexity of the problem*

Any number of electrons ($\leqslant 2j+1$) are allowed in shells with $j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$ but not more than two electrons in any shell of higher angular momentum. It would be possible to relax this restriction with a more comprehensive package of coefficients of fractional parentage.

The version submitted allows up to 10 orbitals and 30 configurations. The orbitals may be distributed in any manner between the filled shells of the "core" and the open shells in the "peel." Limits in COMMON and DIMENSION statements appear in the long write-up.

*Typical running time*

The time required for the test run is $1\frac{1}{2}$ min on an ICL 1906A, of which $\approx 17$ sec is taken in execution.

*References*

[1] D.A. Liberman, D.T. Cromer and J.T. Waber, Computer Phys. Commun. 2 (1971) 107; 2 (1971) 471.
[2] J.P. Desclaux, D.F. Mayers and F. O'Brien, J. Phys. B Atom. Mol. Phys. 4 (1971) 631.
[3] I.P. Grant, Advan. Phys. 19 (1970) 747.
[4] U. Fano, Phys. Rev. 140 (1965) A67.
[5] L. Armstrong Jr., Phys. Rev. 172 (1968) 12, 18.
[6] A. Hibbert, Computer Phys. Commun. 1 (1969) 359; 2 (1971) 180.
[7] I.P. Grant, Computer Phys. Commun. 4 (1972) 377.
[8] P.G. Burke, Computer Phys. Commun. 1 (1970) 241; 2 (1971) 173.

COMPUTER PHYSICS COMMUNICATIONS 5(1973) 283–293. NORTH-HOLLAND PUBLISHING COMPANY

# SOLUTION OF DIFFERENTIAL EQUATIONS FOR EXCHANGE MATRIX ELEMENTS IN HEAVY PARTICLE COLLISIONS

L.A. PARCELL

*Département de Physique and Centre de Recherches sur les Atomes et les Molécules, Faculté des Sciences,*
*Université Laval, Québec, Canada*

Received 23 October 1972

## PROGRAM SUMMARY

*Title of program*: SOLVE D.E. FOR MATRIX ELEMENTS

*Catalogue number*: AAGU

*Computer*: IBM 370. *Installation*: Université Laval, Quebec, Canada

*Operating system*: OS/370

*Programming language used*: FORTRAN IV

*High speed storage required*: 18K words. *No. of bits in a word*: 32

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card reader, Line printer

*No. of cards in combined program and test deck*: 1494

*Keywords:* Atomic, Exchange Matrix Elements, Heavy Particle Collisions, Impact Parameter Approximation, Linear Coupled Differential Equations.

*Nature of physical problem*

In calculating cross sections for atomic collisions employing the impact parameter approximation, exchange matrix elements arise as coefficients of the differential equations for the transition amplitudes. Their evaluation is complicated by phase factors due to electron transfer momentum. The program calculates a general one-electron two-centre exchange integral in terms of which the matrix elements can be expressed.

*Method of solution*

These general exchange integrals may be found by solving a set of coupled differential equations [1]. The program uses a method described by Parcell [2] where the solutions are expressed in terms of a simple quadrature and which allows a step by step evaluation of the solutions along the collision path.

*Restrictions on the complexity of the problem*

The program restricts the general exchange integral to contain s or p angular functions. It could be extended to higher angular functions.

*Typical running time*

The time required to compute solutions will depend on parameter values, the step interval, and the number of solutions. For the test run with velocity 1.5 a.u., to find the values of 52 functions with at least 7-figure accuracy at 180 points between $t = -30$ and $t = 0$ took 80 sec CPU using the G compiler.

*Unusual features of the program*

The program is written to overcome the effect of certain parameters which, for large values, lead to oscillating factors.

*References*

[1] I.M. Cheshire, Proc. Phys. Soc. (London) 92 (1967) 862.
[2] L.A. Parcell, J. Phys. B5 (1972) 1478.

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COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 294–298. NORTH-HOLLAND PUBLISHING COMPANY

# CALCULATION OF THE RADIAL DISTRIBUTION OF EMITTERS IN A CYLINDRICAL SOURCE

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*Applied Mathematics Division, University of Leuven,*
*Heverlee, Belgium*

Received 1 October 1972

## PROGRAM SUMMARY

*Title of program:* ABELA

*Catalogue number:* ABUE

*Computer:* IBM 370/155. *Installation:* Computing Centre, University of Leuven, Heverlee, Belgium

*Operating system:* OS/370

*Programming languages used:* FORTRAN IV

*High speed store required:* 7495 words. *No. of bits in a word:* 32

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* Card reader; Line printer (for the test run)

*No. of cards in combined program and test deck:* 413

*Keywords:* Plasma Physics, Astrophysics, Radiative Transfer, Emitters, Abel Integral Equation, Least-Squares Approximation, Gauss–Jacobi Quadrature.

*Nature of the physical problem*

This program determines the radial distribution of the emission coefficient from measured spectral intensity distributions emitted by an extended source of radiation. It is assumed that the source is optically thin and axially symmetrical.

*Method of solution*

It is well-known [1–4] that this problem can be solved by inverting the Abel integral equation. Using Clenshaw's method [5] a least-squares polynomial is fitted to the observed radiance. The inversion of this polynomial is then carried out exactly by means of Gauss-Jacobi quadrature. This method of calculation is quite insensitive to small random errors in the data.

*References*

[1] W.L. Barr, Method for computing the radial distribution of emitters in a cylindrical source, J. Opt. Soc. Amer. 52 (1962) 885.

[2] K. Bockasten, Transformation of observed radiances into radial distribution of the emission of a plasma, J. Opt. Soc. Amer. 51 (1961) 943.

[3] C.D. Maldonado, A.P. Caron and H.N. Olsen, New method for obtaining emission coefficients from emitted spectral intensities, J. Opt. Soc. Amer 55 (1965) 1247.

[4] G.N. Minerbo and M.E. Levy, Inversion of Abel's integral equation by means of orthogonal polynomials, SIAM J. Numer. Anal. 6 (1969) 598.

[5] C.W. Clenshaw, Curve fitting with a digital computer, Comp. J. 2 (1960) 170.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 299–303. NORTH-HOLLAND PUBLISHING COMPANY

# A ROUTINE FOR CALCULATING THE FORM-FACTOR AND THE ELECTRICAL RESISTIVITY OF LIQUID N.F.E. METALS

Md. M. ISLAM *
*Department of Physics, Queen Mary College, Mile End Road, London, El 4NS, UK*

Received 29 March 1972
Revised manuscript received 13 December 1972

## PROGRAM SUMMARY

*Title of program*: MUKUL

*Catalogue number*: ACKC

*Computer*: ICL 1904 S, *Installation*: Queen Mary College, Mile End Road, London El 4NS

*Operating system*: GEORGE 2E

*Programming language used*: FORTRAN IV

*High speed store required*: 5120 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*Number of magnetic tape required*: None

*What other peripherals are used*? Card Reader; Line Printer

*Number of cards in combined program and test deck*: 118

*Keywords*: Solid State, Liquid NFE Metal, Form-Factor, Structure Factor, Pseudo-Potential, Phase-Shift, Screening, W.S. Radius, Fermi Energy, Fermi Radius, Scattering, Ion, On-Shell, Dielectric Constant, Resistivity

*Nature of physical problem*

This program computes the "form factor" and the electrical resistivity of a liquid nearly-free-electron metal.

*Method of solution*

Form of the "form factor" within the screened uniform charge model [1] is used. The on-shell matrix elements of the pseudopotential are computed using the Born approximation. Ziman's [2] formula for the electrical resistivity is numerically evaluated by using Simpson's rule.

*Restrictions on complexity of the problem*

In the Born approximation angular momenta $\ell < 10$ are used. In the integration of the resistivity formula, intervals $< 200$ are considered. Otherwise dimensions may be altered to increase the scope of the program.

*Typical running time*

Compile time: 2 sec; Execution of sample data: 2 sec.

*References*

[1] M.A. Ball, J. Phys. C. 2 (1969) 1248.
[2] J.M. Ziman, Phil. Mag. 6 (1961) 1013.

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* On leave from Atomic Energy Centre, Dacca, Bangladesh.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 304–307. NORTH-HOLLAND PUBLISHING COMPANY

# ERRATUM NOTICE

*Title of manuscript:* Computation of total, differential and double differential cross sections for compound nuclear reactions of the type $(a, b)$, $(a, b\gamma)$ and $(a, b\gamma-\gamma)$.
(III) Fortran translations of the Algol programs MANDY and BARBARA.

*Authors:* E. Sheldon, S. Mathur and D. Donati

*Reference:* Computer Physics Communications 2 (1971) 272

*Title of programs:* MANDYF and BARBŶF

*Catalogue numbers:* ABOJ and ABOK

*Title of manuscript:* A procedure for nonlinear least squares refinement in adverse practical conditions

*Authors:* J. Lang and R. Müller

*Reference:* Computer Physics Communications 2 (1971) 79

*Title of program:* NONLINEAR LEAST SQUARES FIT

*Catalogue number:* ABGA

Because of a programming error the subroutine FIT diverges in a special case (reduction of the linearity range because of increase of chi squared). The correction eliminates this error; however, it does not affect the test output.

We would like to thank Mr. B. Geelhood for pointing out this error.

# ERRATUM

W. Forster, A brief survey of numerical methods, Computer Physics Communications 4 (1972) 173–181.

In the heading of the paper, the name of the author was inadvertently spelled as W. FOSTER.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 315–327. NORTH-HOLLAND PUBLISHING COMPANY

# THE LIGHT CURVE OF A VARIABLE STAR SUBJECT TO ORBITAL TIDAL DISTORTION

D. HERBISON–EVANS
*Basser Department of Computer Science, Sydney University, N.S.W. 2006, Australia*

Received 6 February 1973

## PROGRAM SUMMARY

*Title of program:* MAGBIN

*Catalogue number:* AACG

*Computer:* KDF9; *Installation:* SYDNEY UNIVERSITY

*Operating system:* KIDSGROVE

*Programming language used:* ALGOL

*High speed storage required:* 20K words. *No. of bits in a word:* 48

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*What other peripherals are used?* Paper tape reader, line printer

*No. of lines in combined program and test deck:* About 840

*Keywords:* Astrophysics, light curve, tidal distortion, binary star, variable star, non-linear least squares.

*Nature of physical problem*

Given a spectroscopic ephemeris of a double star system suffering tidal distortion, this program finds the inclination of the orbital plane, $i$, and the $r_1/a$ ratio ($r_1$ = primary star radius, $a$ = semi major axis of the orbit) from the variation of brightness with time (the 'light curve'). It also finds the period, $P$, amplitude and phase of the oscillation if one of the stars is variable. It also finds the mean brightness of the star and instrumental changes in this value if the star is observed over several years or with different instruments. This program has been used to analyse in this way some observations on $\alpha$ Virginis [1].

*Method of solution*

Trial values of the six unknown parameters (i.e. mean brightness, 2 steps in this mean, $r_1/a$, $i$ and $P$) together with the spectroscopic ephemeris are used to compute theoretical values of the brightness at the times the star was actually observed. The root mean square (r.m.s.) difference between calculated and observed magnitudes (the residual) is minimised by an adaptive simplex search [2] of the parameter values. At each stage, a linear regression gives the amplitude and phase of the oscillation.

Many of the procedures in the program are the same as those in the program solving a spectroscopic double star orbit [3].

*Typical running time*

On an English Electric KDF9 (floating multiplication 15 μsec) with 1159 observations, each residual takes 3 sec to calculate. The number of residuals required by the simplex minimisation depends critically on the accuracy required and the proximity of the initial parameter values to the best ones.

*Restrictions*

As it stands, the program can only accept up to 1159 observations, although this can easily be altered. It only provides for 2 (consecutive) instrumental jumps. The third order

Newton–Raphson solution to Kepler's equation is used. The orbital light curve is assumed to be dominated by orbital variations in only the primary star. The variable star is assumed to have a sinusoidal light curve of fixed period. The program assumes that there are no eclipses and no reflection effect, and also that brightness changes are small enough to be equal to $-2.5 \log_{10}e$ times their magnitude changes, where $e = 2.718$.

*Unusual features*

The program allows doubtful observations to be rejected, and any subset of the parameters to be searched for a minimum residual. Periodically the program breaks off minimising and lists the best parameters so far, their standard deviations, and the values of $a$, $r$, and the stellar masses derived from these parameters.

At the end of the minimisation, the data is listed with corresponding calculated values of the brightness changes due to the orbit and the oscillation, and a graphical output of the residuals is produced on the line printer. Then the calculated oscillation brightness changes are removed to give an observational orbital light curve, and finally the calculated orbital brightness changes are removed instead to give the observed oscillation light curve.

*References*

[1] R.R. Shobbrook, N.R. Lomb and D. Herbison–Evans, Monthly Notices of the Royal Astronomical Society 156 (1972) 165.
[2] J.A. Nelder and R. Mead, Computer Journal 7 (1965) 308.
[3] D. Herbison–Evans and N.R. Lomb, Computer Physics Commun. 2 (1971) 368.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 328–348. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR THE CALCULATION OF X-RAY REFLECTION INTENSITIES

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and

J.E. KIRWAN*
*Central Technical Services, Reactor Group, U.K.A.E.A., Risley, United Kingdom*

**Received 1 February 1973**

## PROGRAM SUMMARY

*Title of program:* FIREFLY II

*Catalogue number:* AAQB

*Computer:* ICL 4-70; *Installation:* U.K.A.E.A., Risley, U.K.

*Operating system:* 7J

*Programming language used:* FORTRAN IV

*High speed storage required:* 138K bytes. *No. of bits in a byte:* 8

*Is the program overlaid?* No

*No. of magnetic tapes required:* 1

*What other peripherals are used?* Card-reader, line-printer

*No. of cards in combined program and test deck:* 2680

*Keywords:* Crystallography, Intensities, X-ray, Powder, Diffraction, Structure-factor, Crystal-structure

*Nature of physical problem*

The program, FIREFLY II, calculates the intensities of X-ray reflections with especial reference to the powder method. The program is very flexible and allows the intensity of reflections with given Miller indices to be calculated if the unit cell and its contents are specified together with the equipment used and, if necessary, temperature and absorption factors. Provision is made for the comparison of observed and calculated data.

*Method of solution*

The Bragg reflection is calculated by the standard formulae of X-ray diffraction as applied to X-ray powder diffraction.

*Restrictions on the complexity of the problem*

The program can manipulate up to 100 sets of Miller indices, 2000 atoms with coordinates $x_n$, $y_n$ and $z_n$, not greater than 100 atom types, 10 wave lengths and up to 1000 observed intensities and angles.

*Typical running time*

5 seconds for a typical example.

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* Present address: A.E., Cawston House, Cawston, Rugby, U.K.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 349–364. NORTH-HOLLAND PUBLISHING COMPANY

# AN EFFICIENT PARTIAL-WAVE ANALYSER FOR THE ABSORPTION MODEL

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R.W. MOORE
*Physics Department, Westfield College, London NW3, UK*

and

K.J.M. MORIARTY
*Department of Mathematics, Royal Holloway College, Englefield Green, Surrey, UK*

Received 16 November 1972

## PROGRAM SUMMARY

*Title of program* : EPWAAM

*Catalogue number* : AAUF

*Computer* : CDC 6600; *Installation* : University of London

*Operating system* : SCOPE

*Programming languages used* : FORTRAN IV

*High speed store required* : 36,160 words. *No. of bits in a word* : 60

*Is the program overlaid* ? No

*No. of magnetic tapes required* : None

*What other peripherals are used* ? Card Reader; Printer

*No. of cards in combined program and test deck* : 2,583

*Keywords descriptive of problem and method of solution* : Nuclear, High Energy, Absorption Model, *s*-Channel Helicity Amplitudes, Partial-Wave Expansion, Rotation Functions, Elastic Scattering, Differential Cross Section, Spin Density Matrix, Gaussian Quadrature, $\chi^2$ Minimization.

*Nature of the physical problem*

This program is concerned with the phenomenological analysis of high-energy 2-body scattering processes in terms of the absorption model.

*Method of solution*

Rather than employ the impact-parameter representation and the subsequent approximations required by such a procedure, the program expands the *s*-channel helicity amplitudes in exact partial-wave series, modifies the partial-wave amplitudes according to the absorption model prescription and resums the series to obtain the modified amplitudes. These amplitudes may then be compared with experiment by means of differential cross sections, polarizations, spin density matrix elements, etc. The integration to obtain the partial-wave amplitudes is performed by gaussian quadrature. By adding the minimization program MINUITS [2] data-fitting may be performed.

*Restrictions on the complexity of the program*

The number of partial-wave amplitudes which must be explicity calculated increases with the momentum of the beam particles. The program is dimensioned for 30 partial-wave amplitudes. This has been found to be quite adequate for beam momenta up to 30 GeV/*c*.

*Typical running time*

This depends on the number of helicity amplitudes to be calculated and on their complexity. A recent application of this program to calculate a wide range of meson–baryon scattering processes by Adjei et al. [1] involving about 70 partial-wave expansions took approximately 120 sec. When used for minimization the running time will depend on the number of parameters to be determined and on how accurately they are required.

*References*

[1] S.A. Adjei, P.A. Collins, B.J. Hartley, R.W. Moore and K.J.M. Moriarty, A Parameter-Free Reggeized Absorption Model for Meson–Baryon Scattering, Ann. of Phys. (N.Y.) 75 (1973) 405.
[2] CERN Program Library No. D506.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 365–378. NORTH-HOLLAND PUBLISHING COMPANY

# ANALYTIC FORMULATION OF SU(3) VECTOR COUPLING COEFFICIENTS FOR *n* PARTICLES

John M. CASILIO and M.E. NOZ
*Physics Department, Indiana University of Pa., Indiana, Pa. 15701, USA*

Received 15 September 1972

## PROGRAM SUMMARY

*Title of program:* SU(3)VCC

*Catalogue number:* AAWA

*Computer:* IBM 360/40; *Installation:* Indiana University of Pa.

*Operating system:* Disk operating system

*Programming language used:* Fortran IV

*High speed storage required:* 8,178 words. *No. of bits in a word:* 32

*Is the program overlaid?* No

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer

*No. of cards in combined program and test deck:* 817

*Keywords:* Nuclear, SU(3), Projection operator, Matrix element, High energy interaction, Vector coupling coefficient, Wigner coefficient, Racah coefficient, Recoupling coefficient, Isoscalar factor, Symmetry principles, Elliot model

*Nature of the physical problem*

A standard quantum mechanical problem is to combine commuting angular momenta to get simultaneous eigenvectors and eigenvalues of $J^2$ and $J_z$. This program calculates analytically SU(3) vector coupling coefficients for a product of *n* particles.

*Method of solution*

The calculation is done by evaluating the matrix elements of the SU(3) projection operator. This is done by using polynomial techniques. The raising and lowering operators of De Swart [1] are used to formulate the projection operator.

*Restrictions on the complexity of the problem*

The intermediate matrix used in the problem solution may become quite large. Therefore, no problem may be done where the intermediate matrix exceeds the storage capacity of the computer used. In the test run, an intermediate matrix of dimension 10 × 10 was used.

*Unusual features of the program*

The technique employed uses a theorem which says that the projection onto any final state of *n* particles, is exactly equal to the projection onto the one dimensional state of $n + 1$ particles. This greatly simplifies the algebra involved. The resulting formula [2] is in closed form and contains fewer sums than any other to be found in the literature. Also, SU(3) isoscalar factors for *n* particles are obtainable by using only part of the program.

*References*

[1] J.J. de Swart, Rev. Mod. Phys. 35 (1963) 916.

[2] M.E. Noz, Ph.D. thesis, Fordham University, N.Y. (1969), Nucl. Phys. B51 (1973) 309.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 379–389. NORTH-HOLLAND PUBLISHING COMPANY

# NEARLY EXACT CALCULATION OF THE SOLUTION OF THE RADIAL SCHRÖDINGER EQUATION

L. MARQUEZ

*Centre d'Etudes Nucléaires de Bordeaux–Gradignan, IN2P3, 33 – Gradignan, France*

Received 19 May 1972

## PROGRAM SUMMARY

*Title of program:* YUKAWA/RH ** LP D JL 72

*Catalogue number:* AAGN

*Computer:* CDC 6600; *Installation:* Centre de Calcul de Physique Nucléaire de Paris, Paris, France

*Operating system:* Scope 3.2

*Programming languages used:* Fortran

*High speed store required:* 50 000 words. *No of bits in a word:* 60

*Is the program overlaid?* No

*No of magnetic tapes required:* None

*What other peripherals are used?* Card reader, line printer

*No of cards in combined program and test deck:* 400

*Keywords:* Atomic, Nuclear, Scattering, Radial Wave Function, Yukawa, Screened Coulomb, Spherical Bessel Function, Nearly Exact.

*Nature of physical problem:*

There are many problems that one finds in elastic scattering that require the solution of the radial Schrödinger equation. There are also many methods to find this solution, a good summary of these methods is given in a paper by Melkanoff et al. [1]. All these methods introduce a certain amount of error in the calculation and this has for consequence, for instance, that certain amount of the irregular solution is mixed to the regular solution.

In most applications, this error has no significance. However, we encountered a problem for which we wanted to have an accuracy comparable to the capability of the computer.

*Method of solution:*

The Schrödinger equation is put in a form that eliminates the fast variations for the low values of $\rho$.

We begin the solution with the power series of $\rho$. We continue this solution by the Taylor series:

One most know or find two quantities characteristic of the computer. The relative error, $\epsilon_s$, with which the computer can register a number in its memory. The lower capacity, $\epsilon_x$, which is the lowest absolute value of a quantity that the computer can handle. These two constants are integrated in the program to control its execution and to make sure that during all the execution, the operations remain within the capability of the computer.

*Restriction on the complexity of the problem:*

The program has been used to compute the wave functions given by the Yukawa or screened Coulomb potential, the Coulomb potential and for no potential, that is the spherical Bessel functions. The value of $\rho$ varied from a small fraction to several thousands and the value of $l$ varied from $l = 0$ to several thousands.

The program could be modified for any potential provided that such a potential and all its derivatives are continuous.

*References*

[1] M.A. Melkanoff, T. Sawada and J. Raynal, Methods in Computational Physics (Academic Press, New-York) 6 (1966) 1.

COMPUTER PHISICS COMMUNICATIONS 5 (1973) 390–394. NORTH-HOLLAND PUBLISHING COMPANY

# ASSOCIATED LEGENDRE POLYNOMIALS, ORDINARY AND MODIFIED SPHERICAL HARMONICS*

W.J. BRAITHWAITE

*University of Texas, Austin, Texas; Princeton University, Princeton, N.J,*
*and*
*University of Washington, Seattle, Washington, USA*

Received 18 July 1972

## PROGRAM SUMMARY

*Title of program*: LEGENDRE

*Catalogue*: ABME

*Computer*: CDC 6600; *Installation*: University of Texas, Austin, Texas, USA

*Operating system*: CDC Scope

*Programming language used*: FORTRAN IV

*High speed storage required*: 4928 words. *No. of bits in a word*: 60

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card reader, line printer

*No. of cards in combined program and test deck*: 160

*Keywords*: General, Expansion, Representation, Rotation, Deformed, Correlations, Symmetry, Legendre Polynomial, Spherical Harmonic, Partial Wave, Fourier.

*Nature of physical problem*

The package LEGENDRE contains three FUNCTION subprograms which calculate, respectively, Legendre polynomials, ordinary and modified spherical harmonics for partial wave or Fourier expansions.

*Method of solution*

The method of calculation is a forward recurrence in $l(l = m, m+1, \ldots, l_{\max})$ for each $m$, from $m = 0, 1, \ldots, m_{\max}$.

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* Supported in part by the U.S. Atomic Energy Commission.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 395–396. NORTH-HOLLAND PUBLISHING COMPANY

# ERRATUM NOTICES

*Title of manuscript*: Computer simulations of Mössbauer spectra for an effective spin $S = \frac{1}{2}$ hamiltonian

*Authors*: E. Münck, J.L. Groves, T.A. Tumolillo and P.G. Debrunner

*Reference*: Computer Physics Communications 5 (1973) 225

*Title of program*: PARAMAGNETIC MÖSSBAUER SPECTRA

*Catalogue number*: ABMD

*Title of manuscript:* Gamma-Radiation Dosimetry for Arbitrary Source and Target Geometry

*Author:* Lincoln B. Hubbard

*Reference:* Computer Physics Communications 2 (1971) 449.

*Title of program:* DOSE1

*Catalogue number:* ACMG

*Title of manuscript*: A program for calculating the static interaction potential between an electron and a diatomic molecule

*Authors*: F.H.M. Faisal and A.L.V. Tench

*Reference*: Computer Physics Communications 2 (1971) 261.

*Title of program*: STATIC INTERACTION POTENTIAL

*Catalogue number*: ACQW

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 405–415. NORTH-HOLLAND PUBLISHING COMPANY

# A USER'S GUIDE TO FORTRAN PROGRAMS FOR WIGNER AND RACAH COEFFICIENTS OF $SU_3$ *

Yoshimi AKIYAMA ** and J.P. DRAAYER

*Dep. of Physics, The University of Michigan, Ann Arbor, Michigan 48104, USA*

Received 16 February 1973

## PROGRAM SUMMARY

*Title of program*: SU3 WIGNER & RACAH COEFFICIENTS

*Catalogue number*: ACRM

*Computer*: IBM 360/67; *Installation*: The University of Michigan, Ann Arbor, Michigan, USA

*Operating system*: MTS/360

*Programming language used*: FORTRAN IV

*High speed storage required*: $SU_3 \supset SU_2 \times U_1$ Wigner coefficients, 13 008 words
$SU_3$ Racah coefficients, 14 654 words;
$SU_3 \supset R_3$ Wigner coefficients, 14 202 words

$SU_3$ Racah coefficients, 14 654 words. $SU_3 \supset R_3$ Wigner coefficients, 14 202 words

*No. of bits in a word*: 32

*Is the program overlaid?* No.

*No. of magnetic tapes required*: None.

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 2046

*Keywords*: $SU_3$, Wigner coefficient, Racah coefficient, Clebsch–Gordan coefficient, Recoupling coefficient, Isoscalar factor, U-function, Unitary coupling, Unitary recoupling, K-band projection, Hypercharge.

*Nature of physical problem*

$SU_3 \supset SU_2 \times U_1$ and $SU_3 \supset R_3$ Wigner coefficients as well as $SU_3$ Racah coefficients are calculated for arbitrary couplings and multiplicity.

*Method of solution*

A build-up process based on the Biedenharn–Louck prescription for specifying the outer multiplicity is employed to generate $SU_3 \supset SU_2 \times U_1$ Wigner coefficients [1]. $SU_3$ Racah coefficients follow through standard recoupling formulae [2]. $SU_3 \supset R_3$ Wigner coefficients are obtained from the corresponding $SU_3 \supset SU_2 \times U_1$ Wigner coefficients via unitary transformation coefficients relating $SU_3 \supset SU_2 \times U_1$ and $SU_3 \supset R_3$ basis states [3].

*Restrictions on the complexity of the problem*

Factorials $M!$, $M \leq M_{\mathrm{max}} = 32$, and binomial coefficients $\binom{N}{M}$, $M \leq N \leq N_{\mathrm{max}} = 32$, are stored in common. Typically for $SU_3 \supset SU_2 \times U_1$ Wigner coefficients $\Lambda_1 + \Lambda_2 + \Lambda_3 \leq M_{\mathrm{max}}$ whereas for $SU_3 \supset R_3$ Wigner coefficients $\lambda + \mu + L \leq N_{\mathrm{max}}$. The limits $M_{\mathrm{max}}$ and $N_{\mathrm{max}}$ may be altered by modifying one and only one subprogram.

*References*

[1] J.P. Draayer and Yoshimi Akiyama J. Math. Phys., in press.
[2] K.T. Hecht, Nuclear Physics 62 (1965) 1.
[3] J.P. Draayer, Nuclear Physics A129 (1969) 647.

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* Work supported by the U.S. National Science Foundation.

** Present address: Department of Physics, Nikon University, Tokyo, Japan.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 416. NORTH-HOLLAND PUBLISHING COMPANY

# A NEW VERSION OF THE PROGRAM TO COMPUTE THE ASYMPTOTIC SOLUTION OF COUPLED EQUATIONS FOR ELECTRON SCATTERING

Alfred T. CHIVERS
*Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast,*
*Belfast, Northern Ireland*

Received 8 February 1973

## PROGRAM SUMMARY

*Title of program*: ASYM VERSION FOR ICL 1900

*Cataloque number*: ACRK

*Computer*: ICL 1907. *Installation*: Queen's University, Belfast, N. Ireland

*Operating system*: George 2

*Programming language used*: FORTRAN IV

*High speed storage required*: 21 632 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: None

*What other peripherals are used*? Card reader, Line printer

*No. of cards in combined program and test deck*: 1202

*Reference to other published version of this program*:
*Catalogue number*: ACQE; *Title*: ASYM; *Ref. in CPC*: 1 (1969) 88

*Keywords*: Atomic, Electron Scattering, Photoionization, Wave Functions, Coupled Equations, Long Range Potentials, Asymptotic Region, WBK, Threshold.

*Nature of physical problem*

This is a new version of the program by Norcross [1]. The program has been changed to conform with ASA Fortran and to become a compatible unit for use with the atomic scattering packages being run on the Queen's University ICL 1907. The changes are as follows:

(i) Alteration of FORMAT statements for the transfer of text to use the Hollerith field descriptor.

(ii) Removal of the IBM System 360 dependent TYPE statements such as

IMPLICIT REAL*8(A–H, O–Z),

REAL*4V.

(iii) Conversion of the program from double precision to single precision since single precision accuracy on the ICL 1907 is adequate for the program.

(iv) Replacement of the four dimensional array AB by two three dimensional arrays AB1 and AB2.

(v) Replacement of all references to the FUNCTION FACT for computing factorials by a COMMON array GAMM. The factorials are now computed by one call from the driver program to the SUBROUTINE SHRIEK and stored in COMMON.

*Reference*

[1] D.W. Norcross, Computer Phys.Commun. 1 (1969) 88.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 417–429. NORTH-HOLLAND PUBLISHING COMPANY

# A GENERAL PROGRAM TO STUDY THE SCATTERING OF PARTICLES BY SOLVING COUPLED INHOMOGENEOUS SECOND-ORDER DIFFERENTIAL EQUATIONS

N. CHANDRA*

*Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast, Northern Ireland*

Received 22 June 1972

## PROGRAM SUMMARY

*Title of the program*: SCAT

*Catalogue number*: AAGO

*Computer*: ICL 1907. *Installation*: Queen's University, Belfast, N. Ireland

*Operating system*: Executive, ICL 1907

*Programming language used*: FORTRAN IV

*High speed storage required*: 59 712 words. *No. of bits in a word*: 24

*Is the program overlaid*? No

*No. of magnetic tapes required*: 1 (optional)

*What other peripherals are used*? Card reader, line printer, card punch (optional), 2 discs or magnetic tapes

*No. of cards in combined program and text deck*: 2566

*CPC library sub-program used:*
*Catalogue number:* ACRK; *Title:* ASYM VERSION FOR 1900; *Ref. in CPC*: 5 (1973) 416

*Keywords descriptive of problem and method of solution*: Atomic, Molecular, Quantum Chemistry, Closed Shell Orbitals, Electron–Atom, Electron–Molecule, Atom–Atom, Atom–Molecule, Cross Section, Rotational Excitation, Rotational–Vibrational Excitation, Coupled Differential Equations, De Vogelaere, *K*-Matrix, Continuum Wavefunctions, Schrödinger Equation.

*Nature of the physical problem*

Many problems in quantum mechanical scattering theory reduce to the solution of coupled second-order differential equations. Examples include the scattering of electrons by atoms and molecules [1], and the scattering of nucleons by nuclei. The program described in this paper solves a general set of such equations where the user is required to provide the potential matrix. The program also allows inhomogeneous terms to be included [2].

*Method of solution*

The coupled equations are integrated using the De Vogelaere algorithm. Linearly independent solutions are obtained by outward integration from the origin and inward integration from the asymptotic region. A complete set of linearly independent solutions are obtained by matching at some intermediate value of the radius and the *K*-matrix, *S*-matrix and cross-section matrix evaluated [3].

*References*

[1] A.M. Arthurs and A. Dalgarno, Proc. Roy. Soc. A.256 (1960) 540.
[2] P.G. Burke and N. Chandra, J. Phys. B. Atom. Molec. Phys. 5 (1972) 1696.
[3] P.G. Burke and M.J. Seaton, Meth. Computational Phys. 10 (1971) 1.

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COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 430–436. NORTH-HOLLAND PUBLISHING COMPANY

# SIMULATION OF CHEMICAL PROFILES DURING ELECTROTRANSPORT

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Received 1 December 1972

## PROGRAM SUMMARY

*Title of program*: ELECTROTRANSPORT SIMULATION

*Catalogue number*: ACIA

*Computer*: IBM 370/165; *Installation*: The Ohio State University Computer Center

*Operating system*: HASP/0S270

*High-speed store required*: 30.5K words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*Other peripherals used?* Card reader, line printer

*No. of cards in combined program and test deck*: 163

*Keywords*: Solid state, Electrotransport, Electromigration, Electrodiffusion, Chemical profile, Capillary-reservoir technique, Liquid metals.

*Nature of physical problem*

The chemical profiles resulting from electrotransport segregation of the components of a liquid binary alloy are simulated through a repetitive calculation based on the concept of competitive transfer of momentum [1]. The simulation is designed for the experimental capillary-reservoir configuration [2] and has produced chemical profiles which are in agreement with experimental results [3]. The simulation is useful in the selection of alloy systems for study and in making proper adjustments in the experimental parameters to guarantee measurable results. The agreement between simulated and experimental results suggests support for the Epstein–Paskin model for electrotransport in liquid alloys.

*Method of solution*

A single closed end capillary tube is divided into NPART zones. The accumulation of an alloy component in each of the zones is calculated for each small time interval by calculating the divergence of the flux, and the accumulation is followed for as many time intervals as is necessary to simulate the length of a particular experimental run. The composition profile is printed after each minute of simulation.

*Typical running time*

The running time depends on the number of time intervals that are calculated; for less than 108,000 1/6-second time intervals (five hour simulation) the average is about two minutes.

*Unusual features of the program*

The alloy composition of the zones after one simulation can be directly used as input for a namelist of another simulation and so on. The flux at each of the interfaces between the zones and the change in the alloy composition in the entire capillary tube are also printed after each minute of simulation. These quantities are useful for electrotransport analytical techniques.

*References*

[1] S.G. Epstein and A. Paskin, Phys. Lett. 24A (1967) 309.
[2] J.D. Verhoeven, Metall. Rev. 8 (1963) 311.
[3] J.L. Blough, D.L. Olson and D.A. Rigney, Mat. Sci. Eng. 11 (1973) 73.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 437–455. NORTH-HOLLAND PUBLISHING COMPANY

# A FINITE ELEMENT PROGRAM PACKAGE FOR AXISYMMETRIC SCALAR FIELD PROBLEMS

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Received 6 June 1972

## PROGRAM SUMMARY

*Title of program*: AXISYMM–SCALAR–HELMHOLTZ–FINTEL 4
*Catalogue number*: ACSB
*Computer*: IBM 360/75, IBM 370/155; *Installation*: McGill University Computing Centre, Montreal, Canada
*Operating system*: OS/360 with HASP–II
*Programming language used*: FORTRAN IV G
*High speed storage required*: 25K words. *No. of bits in a word*: 32
*Is the program overlaid?* No
*No. of magnetic tapes required*: None
*Other peripherals used?* Card reader, line printer, card punch (optional)
*No. of cards in combined program and test deck*: 3638

*CPC Library subprogram used (optional):*
*Catalogue number*: ACSD; *Title*: GENERATE; *Ref. in CPC*: 5 (1973) 438
*Reference to other published version of this program:*
*Catalogue number:* ACSC; *Title:* AXISYMM – SCALAR – HELMHOLTZ – FINTEL 6; *Ref. in CPC:* 5 (1973) 438

*Keywords*: Plasma physics, Fluid dynamics, M.H.D. , Acoustics, Heat transfer, Laplace, Poisson, Helmholtz, Axisymmetric, Scalar field, Finite element, Electrostatics, Heat transfer.

*Nature of physical problem*

Electric field problems requiring solution to Laplace's or Poisson's equations in cylindrical coordinates with no azimuthal variation (e.g. coaxial cable discontinuities, electron guns, electrostatic lenses); acoustics problems requiring solution to the scalar Helmholtz equation in cylindrical coordinates (e.g. Helmholtz resonators); heat-flow problems, plasma simulations, fluid-flow problems.

*Method of solution*

Laplace's, Poisson's or Helmholtz's equations subject to Dirichlet or homogeneous Neumann boundary conditions are solved by the high-order polynomial triangular finite-element method [1]. The method does not involve iterative procedures of any kind. The solution region is subdivided into triangular subregions (finite elements). Over each element the solution is expressed as a linear combination of a complete set of $N$th order interpolation polynomials. The variationally stationary energy functional associated with the Helmholtz equation is approximated in this way by a matrix quadratic form. Extremization with respect to the unknown coefficients yields a simple, relatively low order matrix equation or matrix eigenvalue equation. The latter are solved by standard methods.

*Restrictions on the complexity of the program*

AXISYMM–SCALAR–HELMHOLTZ–FINTEL 4 accepts up to and including 9 different equipotentials (Dirichlet boundary conditions) and the homogeneous Neumann boundary condition. It provides up to and including 4th order polynomial approximation. Mixed order polynomial approximations and mixed material properties can be accomodated, provided that material discontinuities coincide with interelement boundaries. It is intended for problems of matrix size approximately 100 by 100.

*Typical running times*

The execution times are heavily problem-dependent. Using an IBM 360/75, for example, a coaxial cable discontinuity problem which involved the solution of Laplace's equation using 10 fourth-order elements (overall matrix order 67) required 5 sec of arithmetic execution time. Aspace charge problem which involved the solution of Poisson's equation using 16 second-order and 10 fourth-order elements (matrix order 123) required 12 sec. More than 50% of the arithmetic running times are spent on the solution of the matrix equations. Total timings may therefore be estimated from the known matrix algebra timings for any computer.

*Unusual features of the program*

Data in the BLOCK DATA segment of the program are punched in Z format, a feature of the IBM FORTRAN IV. The BLOCK DATA can be generated in other formats using the program GENERATE which must be suitably modified. It is described in this paper.

*Reference*

[1] P. Silvester and A. Konrad, Axisymmetric triangular finite elements for the Scalar Helmholtz equation, Int. J. Numer. Meth. Eng. 5 (1973) 481–497.

## PROGRAM SUMMARY

*Title of program*: AXISYMM–SCALAR–HELMHOLTZ–FINTEL 6

*Catalogue number*: ACSC

*Computer*: IBM 360/75, IBM 370/155; *Installation*: McGill University Computing Centre, Montreal, Canada

*Operating system*: OS/360 with HASP-II

*Programming language used*: FORTRAN IV G

*High speed storage required*: 45 K words. *No. of bits in a word*: 32

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*Other peripherals used?* Card reader, line printer, card punch (optional)

*No. of cards in combined program and test deck*: 4188

*CPC Library subprogram used (optional);*
*Catalogue number:* ACSD; *Title:* GENERATE; *Ref in CPC:* 5 (1973) 438

*Reference to other published version of this program:*
*Catalogue number:* ACSB; *Title:* AXISYMM – SCALAR – HELMHOLTZ – FINTEL 4; *Ref in CPC:* 5 (1973) 438

*Keywords*: Plasma physics, Fluid dynamics, M.H.D., Acoustics, Heat transfer, Laplace, Poisson, Helmholtz, Axisymmetric, Scalar field, Finite element, Electrostatics, Heat transfer.

*Nature of physical problem*

This program is similar to AXISYMM–SCALAR–HELMHOLTZ–FINTEL 4.

*Restrictions on the complexity of the program*

AXISYMM–SCALAR–HELMHOLTZ–FINTEL 6 accepts up to and including 9 different equipotentials (Dirichlet boundary conditions) and the homogeneous Neumann boundary condition: it provides up to and including 6 th order polynomial approximation and is intended for problems of matrix size approximately 200 by 200.

## PROGRAM SUMMARY

*Title of program*: GENERATE

*Catalogue number*: ACSD

*Computer*: IBM 360/75, IBM 370/155; *Installation*: McGill university Computing Centre, Montreal, Canada

*Operating system*: OS/360 with HASP-II

*Programming language used*: FORTRAN IV G

*High speed store required*: 25 K words. *No. of bits in a word*: 32

*Is the program overlaid?* No
*No. of magnetic tapes required*: None
*Other peripherals used?* Card reader, line printer, card punch
*No. of cards in combined program and test deck*: 760

*Purpose of the program*

This program reads in the finite element matrices described and given in ref. [1] in integer form and punches out a complete block data subprogram containing these matrices in Z-format. The latter is an IBM Fortran IV G feature which is convenient for compressing vast amount of numerical data.

Users of the AXISYMM–SCALAR–HELMHOLTZ–FINTEL 4 and AXISYMM–SCALAR–HELMHOLTZ–FINTEL 6 finite element programs (CPC catalogue numbers ACSB and ACSC) who are using computers other than the IBM 360 or 370 series, will have to modify GENERATE in order to produce block data compatible with their Fortran IV compiler. Specifically, this involves only the modification of the output format statements in GENERATE.

All the necessary instructions to run GENERATE as it is are contained in the program listing. The test run output is the BLOCK DATA segments incorporated in AXISYMM–SCALAR–HELMHOLTZ–FINTEL 4 and AXISYMM–SCHALAR–HELMHOLTZ–FINTEL 6.

*Typical running times*

On the IBM 360/75 computer it takes less than 30 sec to run GENERATE.

*Reference*

[1] P. Silvester and A. Konrad, Axisymmetric Triangular Finite Elements for the Scalar Helmholtz Equation, Int. J. Numer. Meth. Eng., 5, no. 4 (1973) 481–497.

COMPUTER PHYSICS COMMUNICATIONS 5 (1973) 456–477. NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAM FOR CALCULATING DIFFERENTIAL AND INTEGRAL CROSS SECTIONS FOR QUANTUM MECHANICAL SCATTERING PROBLEMS FROM REACTANCE OR TRANSITION MATRICES *

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*Chemical Physics Program, Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455, USA*

Received 27 October 1972

## PROGRAM SUMMARY

*Title of program:* DCS

*Catalogue number*: ACRL

*Computer*: CDC 6600; *Installation*: University Computer Center of the University of Minnesota

*Operating system*: MOMS

*Programming languages used*: FORTRAN IV

*High speed store required*: 21000 words. *No. of bits in a word*: 60

*Is the program overlaid?* No

*No. of magnetic tapes required*: Zero or one (optional)

*Other peripherals used:* Card reader, line printer

*No. of cards in combined program and test deck:* 2177

*Keywords*: Atomic, Nuclear, Cross-Section, Scattering, Reactance Matrix, Transition Matrix, Scattering Matrix, Racah Coefficient, Clebsch–Gordan Coefficient, Differential Cross Section.

*Nature of the physical problem*

The differential cross sections for general two-body scattering processes involving elastic, inelastic, and rearrangement scattering of an unpolarized beam of elementary or composite particles and an unpolarized target of elementary or composite particles are evaluated from the relevant transition ($T$) matrices using the formulas of Blatt and Biedenharn [1] with Huby's correction [2] of the error of Wigner and Eisenbud. The $T$ matrices or equivalently useful reactance ($R$) matrices, in the total angular momentum representation, must be supplied as data. The program is applicable to scattering of electrons, atoms, and molecules from atoms and molecules in the chemical physics energy range and to the scattering of electrons, protons, etc. from nuclei in the nuclear physics energy range.

*Method of solution*

The $T$ matrix is block diagonal in total angular momentum $J$ and we will call the blocks $\underset{\sim}{T}^J$ or $J$-blocks. Let the rows of $\underset{\sim}{T}^J$ be labeled $\alpha s l$, where $s$ is the intrinsic angular momentum of the channel, $l$ is the relative orbital angular momentum, and $\alpha$ is the collection of quantum numbers (excluding $J$, $s$, and $l$) which completely describe a channel.

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* Research supported in part by the National Science Foundation under research grant no. GP-28684 and by the University Computer Center and the Graduate School of the University of Minnesota.

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From an input set of *J*-blocks, subprogram CROSS calculates the differential cross sections for the $\alpha s \rightarrow \alpha' s'$ processes of interest, and, if necessary, adds these cross sections to obtain an $\alpha \rightarrow \alpha'$ cross section.

The calculation essentially involves a nine-fold sum over angular momenta. The summands involve $Z$ coefficients [2, 3] and Legendre polynomials,which are each evaluated by separate subprograms.

The integral cross section is calculated by numerical integration of the differential cross section using Weddle's rule and the value is checked with the one found using the orthogonality of the Legendre polynomials.

*Restrictions on the complexity of the problem*

Due to the storage presently allocated for $Z$ coefficient calculations, only values of $J$ less than about 80 should be used, but this can easily be changed.

The other restriction restricts the values of angular momentum which may be used in a calculation. For the present program only integer values of angular momentum are allowed; however, the program can calculate cross sections for processes in which spin and orbital angular momentum are separately conserved. In that case, half-integer spin values are allowed.

*Running time*

The test run required 7 sec (CPU time, excluding compilation and load time) on the CDC 6600.

*Unusual features of the program*

The program also finds, for each $l$, and for each total parity, the transition probability PROBL, the opacity function $P_l$ [4], and the contribution $Q_l$ to the integral cross section.

If cross sections are calculated only for processes in which the channel parity [defined as $(-1)^{I+i}$, $s = I + i$] is conserved, only those $T$ matrix elements $T^{J}_{\alpha' s' l'\,;\,\alpha s l}$ for which $(-1)^{I'+i'-I-i} = 1$ are required; i.e., conservation of channel parity may be used to simplify the calculations in these cases.

The program can check to within some tolerance the symmetry of the *J*-blocks.

*References*

[1] J.M. Blatt and L.C. Biedenharn, Rev. Mod. Phys. 24 (1952) 258.

[2] R. Huby, Proc. Phys. Soc. (London) 67A (1954) 1103.

[3] L.C. Biedenharn, J.M. Blatt, and M.E. Rose, Rev. Mod. Phys. 24 (1952) 249.

[4] R.D. Levine, Quantum Mechanics of Molecular Rate Processes (Clarendon Press, Oxford, 1969), p. 221.

COMPUTER PHYSICS COMMUNICATIONS 6 (1973) 9–16. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTER GENERATION OF FEYNMAN DIAGRAMS FOR PERTURBATION THEORY
## II. PROGRAM DESCRIPTION

H.C. WONG and J. PALDUS

*Quantum Theory Group, Department of Applied Mathematics, University of Waterloo,*
*Waterloo, Ontario, Canada N2L 3G1*

Received 24 April 1973

## PROGRAM SUMMARY

*Title of program*: P.T. DIAGRAM GENERATION

*Catalogue number*: AAKH

*Computer*: S 360/75; *Installation*: University of Waterloo

*Operating system*: OS 360-MVT and HASP II

*Programming languages used*: FORTRAN IV

*High speed store required*: 46k bytes. *No. of bits in a byte*: 8

*Is the program overlaid?* No

*No. of magnetic tapes required*: None

*Other peripherals used?* Card reader, printer

*No. of cards in combined program and test deck*: 879

*Keywords*: Atomic, molecular, electronic structure, many-body problem, Goldstone perturbation theory, Green functions, correlation energy, ionization potentials, electron affinities, excitation energies, Feynman diagrams, Goldstone diagrams, Hugenholtz diagrams.

*Nature of physical problem*

Program finds pertinent topologically distinct diagrams of the Hugenholtz type, which are necessary in calculations of correlation energies, ionization potentials and electron affinities, excitation energies and double ionization processes using the field theoretical form of the perturbation theory.

*Method of solution*

Diagrams are conveniently represented as strings of integers and the topological equivalences are represented by appropriate permutations of these integers. All possible diagrams (i.e. strings) are generated and only the so-called "essentially distinct" are retained. The details of the method used are described in part I [1].

*Restriction on the complexity of the problem*

The program is limited to the first four orders of perturbation theory, however, may be easily extended to higher orders if desired.* Only linked, non-Hartree–Fock diagrams are considered and only one time-version is listed for obvious reasons (cf. part I).

*Typical running time*

The CPU time for the calculation of all possible 3rd order vacuum and Green-function diagrams (both p–h and p–p) is ~1 min on an IBM 360/75. The given test example required 0.16 min of CPU time.

*Unusual features of the program*

Either vacuum or Green-function diagrams may be calculated. In the latter case, both particle–hole and hole–hole diagrams are generated and the so called self-energy diagrams are singled out. By leaving out the free line in the self-energy diagrams we get the one-particle Green-function diagrams.

*References*

[1] J. Paldus and H.C. Wong, Computer Phys. Commun. 6 (1973) 1 (Part I).

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* However, the composition of an integer string into a single integer, which speeds up the comparisons, will have to be modified when the number of integers in the string will exceed the allowed integer length.

COMPUTER PHYSICS COMMUNICATIONS 6 (1973) 17–23. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTATION OF S-STATE BINDING ENERGY AND WAVE FUNCTIONS IN A SAXON–WOODS POTENTIAL

J. CUGNON *

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Received 23 May 1973

## PROGRAM SUMMARY

*Title of program*: BSSW

*Catalogue number*: ABGL

*Computer*: IBM 370/155; *Installation*: University of Liege

*Operating system*: MVT-R20.7

*Programming language used*: FORTRAN IV (G)

*High speed storage required:* 1143 words.
*No. of bits in a word:* 32

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer

*No. of cards in combined program and test deck:* 300

*Keywords:* Nuclear s-state, Woods–Saxon potential, Fox–Goodwin method, spectroscopic number, S-matrix.

*Nature of the physical problem*

The program computes the energy and the wave function of the s-state in a Saxon–Woods potential. It can also determine the well depth or radius which fits a given binding energy.

*Method of solution*

The S-matrix for negative energies is obtained analytically using a method given by Bencze [1]. The equation giving its poles is transformed into a real equation whose solutions are the bound state energies. The wave function is obtained by integrating the Schrodinger equation using the Fox–Goodwin method.

*Restrictions on the complexity of the problem*

Only s-states.

*Typical running time*

The running time is 0.2–0.3 sec for the bound state energy alone, 0.8–0.9 sec if the wave function is required.

*Reference*

[1] G. Bencze, Comment. Physico-Mathemat. 31 (1966) 1.

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* Chercheur I.I.S.N.

COMPUTER PHYSICS COMMUNICATIONS 6 (1973) 24–29. NORTH-HOLLAND PUBLISHING COMPANY

# FREUDENTHAL'S INNER MULTIPLICITY FORMULA

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and

Robert E. BECK
*Department of Mathematics, Villanova University, Villanova, Pennsylvania 19085, USA*

Received 4 September 1972

## PROGRAM SUMMARY

*Title of program*: FREUD

*Catalogue number*: AAAA

*Computer*: IBM 370/165: *Installation*: Uni-Coll Corporation

*Operating system*: HASP-II

*Programming language used*: FORTRAN IV

*High speed store required*: 46 807 words. *No. of bits in a word*: 16

*Overlay structure:* None

*No. of magnetic tapes required*: none

*Other peripherals*: Card reader, line printer

*No. of cards in combined program and test deck*: 1024

*Keywords descriptive of problem and method of solution*:
General, Lie algebra, inner multiplicity, representation, Freudenthal's formula, character.

*Nature of the physical problem*

To compute the weight diagram of an irreducible representation $\rho$ of a complex simple Lie algebra. This problem is equivalent to computing the character of $\rho$.

*Method of solution*

The weight system of the representation is generated using Dynkin's algorithm. Inner multiplicities of the dominant weights are computed using Freudenthal's formula. The multiplicities of the non-dominant weights are computed recursively using a method, based on Weyl reflections, of finding equivalent dominant weights.

*Restrictions on the complexity of the problem*

The program handles all Lie algebras of rank $\leq 9$ and representations with fewer than 1,000 weights.

*Typical running times*

$F_4$, highest weight = 0100, 0.38 sec; $A_3$, highest weight = 030, 0.03 sec.

*Unusual features of the program*

Due to the use of Weyl reflections and emphasis on dominant weights, this implementation is more efficient than those reported in [1] and [2]. By removing the I/O, the program can be used as a subroutine in the computation of outer multiplicities. By using the IBM 360 Fortran IV IMPLICIT statement all variables in the program are declared to be integers. When running on computers other than the IBM 360 and 370 series variables not beginning with I to N will have to be declared as type INTEGER.

*References*

[1] V.K. Agrawala and J.G.F. Belinfante, Weight Diagrams for Lie Group Representations: A Computer Implementation of Freudenthal's Algorithms in ALGOL and FORTRAN, BIT 9 (1969) 301–314.
[2] Mark I. Krusemeyer, Determining Multiplicities of Dominant Weights in Irreducible Lie Algebra Representations Using a Computer, BIT 11 (1971) 310–316.

COMPUTER PHYSICS COMMUNICATIONS 6 (1973) 30–37. NORTH-HOLLAND PUBLISHING COMPANY

# NILSSON ORBITS FOR A PARTICLE IN A WOODS–SAXON POTENTIAL WITH $Y_2^0$ AND $Y_4^0$ DEFORMATIONS, AND COUPLED TO CORE ROTATIONAL STATES

B. HIRD

*Physics Department, University of Ottawa, Ottawa, Ontario, Canada*

Received 27 February 1973

## PROGRAM SUMMARY

*Title of Program*: NILSSON ORBITS

*Catalogue number*: ABOV

*Computer*: IBM 360/65; *Installation*: University of Ottawa, OTTAWA, KIN 6N5, Canada

*Operating system*: HASP

*Programming language used*: Fortran IV

*High speed storage required:* 22,000 Words
*No. of bits in a word:* 32

*Overlay structure:* None

*No. of magnetic tapes required*: None

*Other peripherals used:* Card reader, line printer, card punch

*No. of cards in combined program and test deck*: 881

*CPC Library subprograms used:*
*Catalogue number:* ABMA;
*Title:* GEOMETRICAL COEFFICIENT;
*Ref. in CPC:* 1 (1970) 337

*Keywords*: Nuclear, Schroedinger equation, Woods–Saxon, deformation, hexadecapole, energies, expansion coefficient, Nilsson

*Nature of the problem*

The eigenvalues and expansion coefficients of a single nucleon in an axially symmetric potential are obtained for any quadrupole and hexadecapole deformations. The central part of the potential is assumed to have a Woods–Saxon shape, with the derivative of this shape for the spin–orbit and the deformed parts. The rotational excitations of the core are added to the particle states together with all the rotation-particle (RCP) Coriolis terms to generate the band mixed collective excited state spectrum of a deformed odd $A$ nucleus.

*Method of solution*

The hamiltonian is diagonalised in three successive steps. The spherically symmetric part is first diagonalized in a harmonic oscillator basis, using numerically integrated radial matrix elements. The second diagonalization generates the deformed single particle states in a basis of the spherically symmetric eigenstates of the first diagonalization, and, finally, the core and RCP terms are diagonalized in a basis of the deformed states. A reduction in the size of each of the matrices to be diagonalized and the total number of diagonalizations results from separating the problem in this way.

*Restrictions on the complexity of the problem*

The maximum radial quantum number of the harmonic oscillator basis and hence of any of the other basis states is restricted to 13 for odd parity, and to 12 for even parity systems. Deformations are restricted to $Y_2^0$ and $Y_4^0$ shapes. The Woods–Saxon basis which is used in the deformed state diagonalization is truncated to include only eigenstates with energies below +10 MeV. The above restrictions are fairly easy to relax by small changes in the programme. There is no provision for triaxial deformations, or for vibrational degrees of freedom.

*Typical running times*

The radial integrals, which only need to be calculated once for a given Woods–Saxon potential take 160 sec of CPU time with NMAX = 12 or 13. The three diagonalizations, using, for example, all the states of the 1s, 2s–1d and 1g–2d–3s shells takes a further 45 sec.

COMPUTER PHYSICS COMMUNICATIONS 6 (1973) 38–57. NORTH-HOLLAND PUBLISHING COMPANY

# NUMERICAL EVALUATION OF THE FORMAL SOLUTION OF RADIATIVE TRANSFER PROBLEMS IN SPHERICAL GEOMETRIES

D.G. HUMMER , C.V. KUNASZ and P.B. KUNASZ
*Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado 80302, USA*

Received 12 March 1973

## PROGRAM SUMMARY

*Title of program*: TRANSPHERE

*Catalogue number*: AAAB

*Computer*: CDC 6400; *Installation*: University of Colorado Computer Center

*Operating system*: KRONOS

*Programming language used*: FORTRAN IV

*High speed storage required*: 17,400 words for 8 frequencies, 100 radial points and 60 impact parameters; 22,000 words when number of impact parameters is increased to 100.

*No. of bits in a word:* 60

*Overlay structure:* 2 overlays

*No. of magnetic tapes required*: None

*Other peripherals used*: Scratch space on logical units 1, 2, 3, 4; drivers use card reader and line printer.

*No. of cards in combined program and test deck*: 1808

*Keywords:* Radiative transfer, astrophysics, sperical geometry, formal solution of radiative transfer equation, stellar atmospheres, spectral line formation

*Nature of physical problem*

Given the opacity and source function on a discrete grid of radius and frequency points, this program evaluates the formal solution of the radiative transfer equation in a spherically symmetric atmosphere surrounding a central core, which may be hollow or may absorb and emit radiation in any manner specified by the user. In addition to the radiation intensity, the first three moments of the intensity ($J$, $H$ and $K$) and the Eddington factors $K/J$ and $H/J$ are evaluated at radii and frequencies of interest. This program is designed to be used in the variable-Eddington-factor procedure, as employed for spherical transfer problems by Hummer and Rybicki [1].

*Method of solution*

The transfer equation for each frequency of interest is integrated along parallel rays (lines of constant impact parameter parallel to the line of sight) by using a second-order difference operator to replace the second derivative, thus obtaining a system of linear algebraic equations that includes the boundary conditions at the inner and outer radii. The resulting tridiagonal system is solved by gaussian elimination. Cubic splines are used to obtain the second-order difference operator, to evaluate the optical depth from the given opacity, and to evaluate the angle-integrals for the moments of the intensity. The latter operation is performed in a way that does not require large arrays of intensity data to be stored.

*Restrictions on complexity of the problem*

Discontinuities in the input functions or in their first two derivatives will not be accurately represented by the splines, although by properly choosing the impact parameter-radius grid these effects can be minimized. If an opaque radiating core is specified, a discontinuity in the radiation field can be produced at the impact parameter tangent to the core. While in realistic stellar models the distinction between core and shell is artificial and the discontinuity will not appear, there will be problems in which it must be faced. We have found that by carefully choosing the spatial grid, such problems can be satisfactorily solved; alternative procedures are discussed in section 2.4. The source function and opacity are assumed to be isotropic. Very large ($> 10^3$) ratios of outer to inner radii and/or very large ratios between the maximum and minimum opacities at any point ($> 10^5$) may require a prohibitive number of mesh points and may give rise to cancellation problems.

*Typical running times*

For a case with 6 frequencies, 100 radius points and 58 impact parameters, the total execution time (on the CDC 6400) was 26.4 sec, with the actual formal solution requiring 10.4 sec. Of this time, 9.1 sec. was used for computation and 1.3 sec for disc reading. If optical depth increments and quadrature weights have been previously calculated, total execution time drops to 12.8 sec.

*References*

[1] D.G. Hummer and G.B. Rybicki, Monthly Notices Roy. Astr. Soc. 152 (1971) 1.

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COMPUTER PHYSICS COMMUNICATIONS 6 (1973) 59–61. NORTH-HOLLAND PUBLISHING COMPANY

# ERRATUM NOTICE

*Title of manuscript:* A new version of a general program to calculate angular momentum integrals in atomic structure
*Author:* A. Hibbert

*Reference:* Computer Physics Communications 2 (1971) 180
*Title of program:* WEIGHTS NEW VERSION
*Catalogue number:* ACQV

COMPUTER PHYSICS COMMUNICATIONS 6 (1973) 77–87. NORTH-HOLLAND PUBLISHING COMPANY

# PHASE SHIFT ANALYSIS AND CONSISTENCY CHECKS ON ELECTRON–ATOM COLLISION DATA

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*Department of Mathematics, Royal Holloway College, Englefield Green, Surrey, UK*

Received 11 May 1973

## PROGRAM SUMMARY

*Title of program*: SHIFTA

*Catalogue number*: AAGV

*Computer*: CDC 6600; *Installation*: ULCC

*Operating system*: SCOPE

*Program language used*: FORTRAN IV

*High-speed storage required*: 11667 words
*No. of bits in a word:* 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards and combined program and test deck*: 2018

*Keywords*: Atomic, scattering, electron, partial wave, phase-shift analysis, non-relativistic.

*Nature of physical problem*

The program tests the consistency of different sets of experimental measurements of electron-atom scattering below the first inelastic threshold and indicates the relative merit of each measurement. The program produces a set of parameters which give values of the first $l_0$ phase shifts (subject to certain specified constraints) consistent with the data.

*Method of solution*

Theoretical expressions for the experimental quantities are obtained in terms of the partial wave phase shifts for elastic scattering. The first $l_0$ phase shifts are parametrized, the remainder being obtained in Born's approximation, and a minimization subroutine is used to simultaneously fit the (parametrized) values to all the selected experimental measurements.

Starting with an initial set of parameters based on theoretical estimates of the scattering length and of the first $l_0$ phase shifts throughout the elastic region, the minimisation subroutine produces a new set of 'best fit' parameters which are then used to recalculate the first $l_0$ phases, subject to constraints of continuity, unitarity, and effective range formulae requirement near zero energy.

These 'best fit' phases for $l \leqslant l_0$, and the corresponding Born phases for $l > l_0$, are used to provide 'best fit' values, $X$, corresponding to each piece of experimental data, $x_i$, to which an estimated error $\delta x_i$ is attached. If the corresponding value $\chi_i^2 = [(X_i - x_i)/\delta x_i]^2$ is large compared with the mean value of $\chi^2$ for all the data, the assigned $\delta x_i$ for this piece of data is likely to be too small.

*Restrictions on the complexity of the problem*

The program in this version is restricted to analysis of certain types of experiments only, viz

a) total elastic cross-sections;
b) differential elastic cross-sections;
c) diffusion cross-sections;
d) total cross section measurements expressed via a dispersion relation in terms of $\mathrm{Re}\, f(0, E)$.

Measurements of (a), (b), (c) and (d) at the same $N_1$ ($\leqslant 16$) energy values, together with a further $N_2$ ($\leqslant 34$) values of (c) at other energies, may be used. Differential cross-sections at each of the $N_1$ energies at $N_3$ ($\leqslant 15$) different angles may be handled.

Independent sets of measurements of any of (a) to (d) can be treated simultaneously by duplication of the appropriate subroutine (e.g. QTOTAL → QTOTA 1 and QTOTA 2) and call statement.

*Typical running time*

On a CDC 6600, a typical average running time would be about 15 sec per iteration, depending on the values of $N_1$, $N_2$, and $N_3$.

COMPUTER PHYSICS COMMUNICATION 6 (1973) 88. NORTH-HOLLAND PUBLISHING COMPANY

# A NEW VERSION OF THE PROGRAM TO COMPUTE THE FRACTIONAL PARENTAGE COEFFICIENTS FOR EQUIVALENT d SHELL ELECTRONS

Alfred T. CHIVERS
*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, Northern Ireland*

Received 12 June 1973

## PROGRAM SUMMARY

*Title of program*: A NEW D SHELL CFP

*Catalogue number*: ACRN

*Computer*: ICL 1907; *Installation*: Queen's University, Belfast, N. Ireland.

*Operating system*: George 2

*Programming language used*: FORTRAN IV

*High speed storage required*: 5312 words.

*No. of bits in a word*: 24

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 412

*Reference to other published version of this program*:
*Catalogue number*: ACQC
*Title*: D SHELL C.F.P.
*Ref in CPC*: 1 (1969) 15

*Keywords*: Atomic, nuclear, Racah C.F.P.

*Nature of the physical problem*

This is a new version of the program by Allison [1]. The program has been changed to conform with ANSI Fortran and to use a Block Data Subprogram for the data. The changes are as follows:

(1) The integer constant referring to the channel number in the WRITE statements in the directing program has been replaced by an integer variable which is transmitted to subprogram CFPD in the COMMON block INFORM.
(2) Some non-standard Fortran statements have been replaced in the directing program.
(3) A BLOCK DATA subprogram has been inserted resulting in the removal of the non-standard READ statements in the subprogram CFPD. The data is now transferred through the COMMON BLOCK FRPAR2. This facilitates the use of the subprogram in larger program packages, for example [2,3].

*References*:

[1] D.C.S. Allison, Computer Phys. Commun. 1 (1969) 15.
[2] A. Hibbert, Computer Phys. Commun. 2 (1971) 180.
[3] W.D. Robb, Computer Phys. Commun. (to be published).

COMPUTER PHYSICS COMMUNICATION 6 (1973) 89–95. NORTH-HOLLAND PUBLISHING COMPANY

# ATOMIC INTEGRAL CONTAINING THREE ODD POWERS OF INTERELECTRONIC SEPARATION COORDINATES

A.H. MOUSSA* and H.M.A. RADI
*Department of Physics, University of Kuwait, Kuwait*

Received 17 May 1973

## PROGRAM SUMMARY

*Title of program*: ATOMINT

*Catalogue number*: ACRO

*Computer*: IBM 360/30

*Installation*: Planning Board, Kuwait

*Operating system*: SYSTEM/360 (DOS)

*Programming languages used*: FORTRAN IV

*High speed store required*: 71,847 bytes

*No. of bits in a byte*: 8

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, printer

*No. of cards in combined program and test deck*: 458

*Keywords*: Atomic, bound state, scattering, Hylleraas functions, variational method

*Nature of physical problem*

The subroutine ATOMINT evaluates an atomic integral, containing 3 odd powers of interelectronic separation coordinates, which appears in bound state variational calculations of three electron atoms, and in phase shift variational calculations of scattering of electrons (or positrons) by two-electron atoms.

*Method of solution*

The integral is expanded as infinite sums of Legendre polynomials, and these angular terms are reduced, by applying the coupling rules of spherical harmonics, to simple integrals which are easily integrated. The orthogonal properties keep one infinite sum only to do. The limits of the radial integrals are divided into six parts, and the resulting integrals are evaluated in closed forms in most cases and in a convergent sum in one case. On the average, five terms lead to a reasonable accuracy.

*Typical running time*

The time depends on the input values, and on the number of terms in the infinite sum; the average time is between 5 – 10 min approximately.

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## ERRATUM

I.P. Grant, A general program to calculate angular momentum coefficients in relativistic atomic structure, Computer Physics Communications 5 (1973) 263–282.

P. 278. The second line of eq. (18) should read

$$= n_1 n_2 \sum_{J'=|j_1-j_2|}^{j_1+j_2} [(2J'+1)/(2j_1+1)(2j_2+1)]\, V(j_1 j_2 J')\,.$$

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COMPUTER PHYSICS COMMUNICATION 6 (1973) 99–131. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTATION OF TOTAL AND DIFFERENTIAL CROSS SECTION FOR COMPOUND NUCLEAR REACTIONS OF THE TYPE (a, a), (a, a′), (a, b), (a, $\gamma$), (a, $\gamma$-$\gamma$), (a, b$\gamma$) AND (a, b$\gamma$-$\gamma$).

## (IV) FORTRAN PROGRAM 'CINDY'

E. SHELDON and V.C. ROGERS
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*and*
*Physics Department, Brigham Young University, Provo, Utah 84601, USA*†

Received 15 June 1973

## PROGRAM SUMMARY

*Title of program:* CINDY

*Catalogue number:* ABMF

*Computer:* IBM 370/165 and/or IBM 360/50.

*Installation:* MIT Information Processing Center and Brigham Young University Computer Research Center.

*Operating system:* FORTRAN – IV G, Level 20/21

*Programming languages used:* FORTRAN–IV

*High speed store required:* 30 K words. No. of bits in word: 36

*Overlay structure:* None

*No. of magnetic tapes required:* None.

*Other peripherals used:* Card reader; Line printer

*No. of cards in combined program and test deck:* 2367

*Reference to other published versions of this program:*

| *Catalogue number* | *Title* | *Ref in CPC* |
|---|---|---|
| ABOA | MANDY | 1 (1969) 35 |
| ABOJ | MANDYF | 2 (1971) 272 |

*Keywords:* Nuclear, reaction mechanism, angular distribution, compound nucleus, statistical model, differential cross section, total cross section, radiative capture, continuum, energy levels, spin-parity assignments, multipolarity, mixing ratio, optical model, compound-elastic scattering, inelastic scattering, compound stripping, transfer reactions, Hauser–Feshbach, Satchler, Moldauer, level-width fluctuation, Weisskopf, radiative widths.

*Nature of physical problem*

Evaluation of total and differential cross sections in absolute and normalized form for (a, a), (a, a′), (a, b), (a, $\gamma$), (a, $\gamma$-$\gamma$), (a, b$\gamma$) and (a, b$\gamma$-$\gamma$) processes in $j-j$ coupling formalism using statistical compound-nucleus theory, with spin–orbit interaction and/or the Moldauer level-width fluctuation correction if desired. As a generalization of its predecessor, "MANDYF" [1], the program has been extended to cater for radiative capture (in observed or competing transitions), to take account of competing channels to a continuum of residual states, and to automatically calculate any required transmission coefficients from prespecified optical-potential parameters. It is capable of furnishing data for twin-level resonance calculations [2] and evaluating magnetic substate populations [3] from $\gamma$-distribution parameters.

*Method of solution*

Akin to "MANDYF" [1], but with modified organization, the program tabulates momenta permitted by selection rules, calculates penetrabilities, and builds products of these with appropriate Racah factors to generate Legendre-polynomial expansion coefficients. Thence total and differential cross sections are evaluated in absolute and normalized form automatically.

*Restrictions on the complexity of the problem*

Dimensional restrictions commensurate with storage capacity dictate that incoming and outgoing orbital momenta be $\ell \leqslant 8$ and the number of extra channels be O3 $\leqslant 40$ in the present version (readily capable of extension).

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† Work supported in part by the National Science Foundation.

*References*

[1] E. Sheldon, S. Mathur and D. Donati, Computer Phys. Commun. 2 (1971) 272;
See also E. Sheldon and R.M. Strang, Computer Phys. Commun. 1 (1969) 35.

[2] A.D. Robb, W.A. Schier and E. Sheldon, Nucl. Phys. A147 (1970) 423;
E. Sheldon, W.A. Schier, G.P. Couchell, B.K. Barnes, D. Donati, J.J. Egan, P. Harihar, S.C. Mathur and A. Mittler, in *Statistical Properties of Nuclei,* (ed. J. Garg), Plenum Publ. Corp., N.Y., (1972) p. 121.

[3] E. Sheldon, V.C. Rogers and D. Donati, Bull. Am. Phys. Soc. 17 (1972) 167, Paper B4;
E. Sheldon and D. Donati, Bull. Am. Phys. Soc. 18 (1973) 649, Paper GH 7;

COMPUTER PHYSICS COMMUNICATION 6 (1973) 132–148. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM TO EVALUATE THE REDUCED MATRIX ELEMENTS OF SUMMATIONS OF ONE-PARTICLE TENSOR OPERATORS

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*BOULDER, Colorado 80302, USA*

Received 10 October 1972

## PROGRAM SUMMARY

*Title of program*: REDUCED TENSOR MATRIX ELEMENTS

*Catalogue number*: AAKF

| *Computer*: | *Installation*: |
|---|---|
| ICL 1907 | Queen's University, Belfast |
| CDC 6600 | University of London, England |
| IBM 360/75 | Centre Européen de Calcul Atomique et Moléculaire, 91-Campus d'Orsay, France |

*Operating system*: GEORGE II

*Programming languages used*: FORTRAN

*High speed store required*: 21056 words

*No. of bits per word*: 24

*Overlay structure*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1094

*CPC Library subprograms used*:

| *Catalogue numbers* | *Titles* | *Refs. in CPC* |
|---|---|---|
| ACQB | P SHELL CFP | 1 (1969) 15 |
| ACRN | A NEW D SHELL CFP | 6 (1973) 88 |
| AAGD | NJSYM | 1 (1970) 241 |
| AAGD0001 | ADAPT NJSYM FOR WEIGHTS | 2 (1971) 180 |

*Keywords*: Atomic, nuclear, transitions, electric multipole, magnetic multipole.

*Nature of the physical problem*

The calculation of many nuclear and atomic properties depends on the evaluation of matrix elements of summations of one-particle tensor operators.

The program TENSOR enables one to calculate such matrix elements of any spin-dependent or spin-independent one-particle tensor operator, between arbitrarily coupled L–S configurations.

*Method of solution*

The notation, and phase convention, of Fano [1] is used to obtain programmable expressions for the matrix element in terms of spin and orbital recoupling coefficients and coefficients of fractional parentage. However the results produced by the program are independent of the phase convention adopted for the tensor operator.

*Restrictions on the complexity of the program*

The program assumes that both configurations are formed from the same orthonormal set of basis orbitals, and that the angular momenta of the shells in each configuration are coupled successively. Further we are restricted by the available fractional parentage routines to p- and d-shells and at most two particles in higher shells. However this restriction can be removed by the introduction of appropriate f-, g-shell etc. fractional parantage routines.

*Typical running time*

For the test data provided the program required 57 sec of ICL 1907 CPU time for execution.

*Reference*

[1] U. Fano, Phys. Rev., 140 (1965) 67.

COMPUTER PHYSICS COMMUNICATION 6 (1973) 149–155. NORTH-HOLLAND PUBLISHING COMPANY

# IRREDUCIBLE MULTIPLIER REPRESENTATIONS☆

T.G. WORLTON
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Received 12 March 1973

## ADAPTATION SUMMARY

*Title of adaptation*: IMR CALCULATION

*Adaptation number*: 0002

*Reference to original program:*
*Cat. No.:* ACMI; *Title:* GROUP THEORY OF LATTICE DYNAMICS; *Ref.:* CPC 3 (1972) 88

*Authors of original program:* T.G. Worlton and J.L. Warren

*Computer:* IBM 370–195; *Installation:* Argonne National Laboratory

*Operating system:* OS 370 MVT

*Programming language used in adapted program:* FORTRAN IV

*High speed storage required:* 50K words

*No. of bits in a word:* 32

*No. of cards required to effect adaptation (including directive cards):* 532

*Additional keywords:* Irreducible multiplier representations, ray representations, factor system, coset composition

*Nature of physical problem*
The adaptation inserts a subroutine to generate irreducible multiplier representations of the group of the wave vector $G_0(\boldsymbol{k})$. In the original version of ACMI [1] these quantities were read from cards.

*Method of solution*
IMR's of $G_0(\boldsymbol{k})$ are induced from those of a subgroup of prime order starting from an invariant cyclic subgroup [2].

*Restrictions on the complexity of the problem*
The program would have to be modified for double groups.

*Typical running time:* 1 sec.

*Unusual features of the program*
Although designed to improve the program ACMI, this new subroutine together with some subroutines from ACMI can be used as an independent program to calculate IMR's.

The present adaptation can be used in addition to ACMI0001 for analysis of external modes of molecular crystals [3].

*References*

[1] T.G. Worlton and J.L. Warren, Computer Phys. Commun. 3 (1972) 88.
[2] V.C. Sahni and G. Venkataramen, Phys. Kond. Mat. 11 (1970) 199.
[3] T.G. Worlton, Computer Phys. Commun. 4 (1973) 249.

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☆ Based on work performed under the auspices of the U.S. Atomic Energy Commission.

COMPUTER PHYSICS COMMUNICATIONS 6 (1973) 165–186. NORTH-HOLLAND PUBLISHING COMPANY

# DIRAC
# DYNAMIC INFORMATION RETRIEVAL OF ATOMIC CODES☆
## II. IMPLEMENTATION

Alan R. DAVIES†, Kenneth SMITH★ and K.L. KWOK
*Behlen Laboratory of Physics, University of Nebraska, Lincoln, Nebraska 68508, USA*

Received 30 May 1972

## PROGRAM SUMMARY

*Title of program:* DIRAC

*Catalogue number:* AAIB

| *Computer:* | *Installation:* |
|---|---|
| IBM 360/65 | University of Nebraska |
| IBM 360/91 | Goddard Space Flight Center |

*Operating system:* OS/360 – MVT

*Programming language used:* FORTRAN

*High speed storage required:* 200K bytes

*No. of bits in a byte:* 8

*Overlay structure:* Overlaid

*No. of magnetic tapes required:* None

*Other peripherals used:* IBM 2250 graphics display device with light pen, an alphameric keyboard and a programmed function keyboard, IBM 2321 Data Cell and an IBM 2314 Disc Unit.

*No. of cards in combined program and test deck:* 9320

*CPC Library subprograms used:*
*Catalogue number:* AAIC;
*Title:* DATBNK;
*Ref. in CPC:* 6 (1973) 166

*Keywords:* Atomic, collision, cross section, electron scattering, graphical display, information retrieval, interactive, photoionization.

*Nature of physical problem*

DIRAC (dynamic information retrieval of atomic codes) is a program which dynamically retrieves information from a databank upon a users request and displays this information on an on-line 12" × 12" graphical display unit (IBM 2250). The display can be tabular or graphical of any of the data stored in the databank. The databank is itself formed by Dirac and is automatically updated if runs are initiated by the user from the display unit. The system can be used by any collection of theoretical codes for calculating cross sections; experimental points can also be fed into the databank.

*Method of solution*

A user sits in front of the graphics display unit with an alphameric keyboard and with the use of a light pen and programmed function keyboard buttons is taken through a selection procedure by interacting with the display frames appearing on the unit. The atomic collision physics problem of interest to the user is built up by selecting the appropriate constants of the problem. Finally the answers to the problem can be displayed graphically or tabularly if they exist *or* if they do not exist, new runs can be instigated using codes like SEBAS [1] and ATOMNP [2] to produce the new data. A complete description of the user options is given in a first paper [3].

*Restrictions on the complexity of the problem*

Data is in the form of discrete points which can be plotted on a rectangular set of axes where the absissa is always taken to be the energy (except for differential cross sections which is in radians) and the ordinate is the physical data.

The fundamental restrictions are defined in the design characteristics of the directories. In general terms, these are determined by the rules of L–S coupling in collision processes.

*Typical running time*

As the program is run in an interactive mode with the user in front of the graphics device then the analysis of existing data takes place in real time. Retrieving the complete physics data for several hundred points takes of the order of 10 se-

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☆ Work supported by the National Science Foundation

† Department of Computer Science, Royal Holloway College, Egham, Surrey, UK.

★ Centre for Computer Studies, University of Leeds, UK.

conds. Plotting these points and drawing the curves on the screen takes of the order of 10 seconds. The computation and plotting of resonance shapes is immediate.

*Unusual features of the program*

The entire memory hierarchy (core, disc, data cell and magnetic tape) is used dynamically by Dirac to optimize its use of the computer resources. A routine is incorporated into DIRAC by which the user can initiate runs of the computer codes, which updates the data bank, directly from the "physics frames".

To run this program on other manufacturer's equipment will require the user to supply equivalent routines to those taken from the IBM graphic subroutine package [4].

*References*

[1] K. Smith and L.A. Morgan, Phys. Rev. 165 (1968) 110.

[2] M.J. Conneely, L. Lipsky, K. Smith, P.G. Burke and R.J.W. Henry, Computer Phys. Commun. 1 (1970) 306–324.

[3] A.R. Davies, K. Smith and K.L. Kwok, DIRAC–Dynamic Information Retrieval of Atomic Codes 1. Physical Design Criteria. Computer Phys. Commun. 3 (1972) 277–295.

[4] IBM System/360 Operating System, Graphic Programming Services for FORTRAN IV – Form C27-6932-2.

## PROGRAM SUMMARY

*Title of program:* DATBNK

*Catalogue number:* AAIC

| *Computer:* | *Installation:* |
|---|---|
| IBM 360/65 | University of Nebráska. |
| IBM 360/91 | Goddard Space Flight Center |

*Operating system:* OS/360-MVT

*Programming language used:* FORTRAN

*High speed storage required:* 120K bytes

*No. of bits in a byte:* 8

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer, IBM 2314 disc unit

*No. of cards in combined program and test deck:* 7128

*Nature of physical problem*

The program DATBNK is a small FORTRAN program which reads in test data from cards and stores it in the data bank files on disc ready for use by DIRAC. This data is written onto seven direct access files. The test run of DIRAC assumes this data is already in the disc files in the form of direct access files.

The data included with the program is for the targets S+, N+ and O+ and consists of 6945 cards. This test data defines the targets, the atomic codes producing the data, the physical model, the $LS\pi$ of the model, the energies, the raw data for each target (e.g. R matrics, cross sections etc.) and the physics reference table.

COMPUTER PHYSICS COMMUNICATION 6 (1973) 187–193. NORTH-HOLLAND PUBLISHING COMPANY

# KRAMERS–KRONIG ANALYSIS OF REFLECTION DATA

R. KLUCKER [☆] and U. NIELSEN [★]

*Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany*

Received 30 March 1973

## PROGRAM SUMMARY

*Title of program*: KRKAN

*Catalogue number*: ACKD

*Computer*: IBM 360/75 or IBM 360/65; *Installation*: Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

*Operating system*: OSMVT/Release 21.6

*Programming languages used*: FORTRAN IV

*High speed store required*: 64 kbytes

*No of bits in a byte*: 8

*Overlay structure*: None

*No of magnetic tapes required*: None

*Other peripherals used*: Card reader (unit 5); line printer (unit 6)

*No of cards in combined program and test deck*: 583.

*Keywords*: Solid state physics, dispersion-relation, Kramers–Kronig integral, radiation, reflectance, optical constants, dielectric constants

*Nature of physical problem*

Optical and dielectric constants of insulators and semiconductors are calculated from reflectance spectra using the Kramers–Kronig dispersion relation [1]

$$\mathrm{Im} f(\omega_k) = -\frac{2\omega_k}{\pi} \int_0^\infty \frac{\mathrm{Re} f(\omega)}{\omega^2 - \omega_k^2}\,\mathrm{d}\omega. \tag{1}$$

$\mathrm{Im} f(\omega)$, $\mathrm{Re} f(\omega)$ are the imaginary and the real part of the complex function $f(\omega)$, respectively [e.g. $f(\omega) = \hat{\epsilon}(\omega) = \epsilon_1(\omega) + \mathrm{i}\epsilon_2(\omega)$].

*Method of solution*

Since reflectance spectra are only available in a restricted frequency range, say between $\omega_\ell$ and $\omega_\mathrm{u}$, the integral of eq. (1) is split into 3 parts:

$$\int_0^\infty = \int_0^{\omega_\ell} + \int_{\omega_\ell}^{\omega_\mathrm{u}} + \int_{\omega_\mathrm{u}}^\infty = I_{0\ell} + I_{\ell\mathrm{u}} + I_{\mathrm{u}\infty}.$$

$I_{0\ell}$ and $I_{\mathrm{u}\infty}$ are evaluated by assuming physically reasonable extrapolation functions: 1. For $0 \leqslant \omega \leqslant \omega_\ell$ $\mathrm{Re} f(\omega) = \mathrm{Re} f(\omega_\ell)$ is assumed. 2. For $\omega > \omega_\mathrm{u}$ the electrons of the material are treated as a free electron gas. For $\omega_\ell \leqslant \omega \leqslant \omega_\mathrm{u}$ $\mathrm{Re} f(\omega)$ is expanded within small intervals to powers of $\omega$ (up to some degree $m$). Then $I_{\ell\mathrm{u}}$ is evaluated by using these approximations and by summation over all intervals.

*Restriction on the complexity of the problem*

This program computes optical and dielectric constants only from reflectance spectra which are obtained with polarized light, the electrical field vector of which is lying either perpencidular or parallel to the plane of incidence.

For the integration only the linear term of the expansion of $\mathrm{Re} f(\omega)$ is used. But according to the long write-up this program may easily be modified if higher approximations are desired.

*Typical running time*

Typical rumming time is about 50 sec on the IBM 360/75 for one set of data and an output of 6000 lines printed.

*Unusual features of the program*

This program is especially suited to accept data in the form of punched cards from a card punching machine (IBM 024). The original curves are converted by means of a $X-Y$-recorder with retransmitting slidewire potentiometers and an analog-digital converter connected to this punching machine [2].

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[☆] Sektion Physik, Universität München, München, Germany. Now with: Scientific Control System GmbH, Hamburg, Germany.

[★] II. Institut für Experimentalphysik, Universität Hamburg, Hamburg, Germany.

*References*

[1] D.M. Roessler, Brit. J. Appl. Phys. 16 (1965) 1359.

[2] B. Sonntag, Thesis, University of Hamburg, Hamburg, Germany (1969).

COMPUTER PHYSICS COMMUNICATIONS 6 (1974) 221–228. NORTH-HOLLAND PUBLISHING COMPANY

# A FAST QUADRATURE METHOD FOR COMPUTING DIATOMIC RKR POTENTIAL CURVES

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*Lab. of Molecular Structure and Spectra, Dep. of Physics,*
*University of Chicago, Chicago, Illinois 60637, USA*

Received 30 July 1973

## PROGRAM SUMMARY

*Title of program*: RKRPOT

*Catalogue number*: AAEE

*Computer*: IBM 370/168; *Installation*: University of Chicago Computer Center, Chicago, Illinois 60637

*Operating system*: HASP/OS/MVT

*Programming language used*: FORTRAN IV

*High speed storage required*: 9104 words.

*No. of bits per word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, card punch

*No. of cards in combined program and test deck*: 251

*Keywords*: Molecular, diatomic, potential curves, RKR method, gaussian quadrature.

*Nature of physical problem*
The RKR method provides a prescription for computing diatomic potential curves from empirical spectroscopic parameters. The right- and left-hand turning points on the curve are related to the spectroscopic quantities through the Klein $f$ and $g$ integrals [1]. The heart of the problem is the evaluation of these improper integrals.

*Method of solution*
The $f$ and $g$ integrals are obtained by numerical integration, using a very efficient Gauss–Mehler quadrature with weight function $(1-x)^{-1/2}$ on the interval $(-1, 1)$ [2]. For vibrational levels having energy less than ~ 80% of the dissociation energy $D_e$, a 4-point quadrature typically yields an accuracy of 1 part in $10^7$.

*Restrictions on the complexity of the problem*
As written, the program computes the vibrational energy $G(v)$ and rotational constant $B(v)$ from the conventional polynomial expressions for these quantities, with the expansion parameters provided as input. However, the appropriate function routines could be modified easily to include, for example, a mode for interpolating on the raw spectroscopic quantities.

*Typical running time*
For vibrational levels satisfying the condition, $G(v) \lesssim 0.8\,D_e$, the integral estimates usually converge in two cycles, in which case the program will compute the turning points for each level in 5–10 msec, depending on the number of vibrational and rotational expansion parameters. As the levels approach the dissociation limit, the convergence rate decreases markedly, taking as much as ~ $\frac{1}{3}$ sec for levels within ~ 1 cm$^{-1}$ of $D_e$.

*References*

[1] O. Klein, Z. Phys. 76 (1932) 226.
[2] J. Tellinghuisen, J. Mol. Spectrosco. 44 (1972) 194.

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[☆] Present address: NOAA, Environmental Research Laboratories, U.S. Dep. of Commerce, Boulder, Colorado 80302, USA.

COMPUTER PHYSICS COMMUNICATION 6 (1974) 229–239. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM CALCULATING THE FORMULAE FOR POLARIZATION EFFECTS IN NUCLEAR REACTIONS

F. SEILER

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*Klingelbergstrasse 82, CH-4056 Basel, Switzerland*

Received 3 September 1973

## PROGRAM SUMMARY

*Title of program*: FATSO

*Catalogue number*: ABGM

*Computer*: UNIVAC 1108; *Installation*: Sandoz AG, Basel, Switzerland

*Operating system*: EXEC 8

*Programming language used*: FORTRAN IV

*High speed store required*: 44030 words. *No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1835

*Keywords*: Nuclear, polarization, tensor moments, reaction matrix, cross-section, polarization efficiencies, correlation coefficients, polarization transfer.

*Nature of physical problem*

In nuclear reactions involving two particles in both the incoming and outgoing channel, the experimentally observable quantities (cross-sections, polarizations, etc.) can be parametrized in terms of the reaction matrix $R$. The properly normalized observables can be expanded in terms of rotation matrices $d^{(L)}_{m'm}(\theta)$ or Legendre functions $P_{L,q}(\cos\theta)$ depending on the symmetries involved. The corresponding expansion coefficients are then bilinear functions of the reaction matrix elements $\langle l's'J^{\pi}|R|lsJ^{\pi}\rangle$ in the $(l, s, J)$ coupling scheme. The numerical factor for each bilinear combination of matrix elements in a given coefficient is a complicated function involving Clebsch–Gordan, Racah and X-coefficients.

*Method of solution*

The algebraic expressions for the numerical factors have been given by several authors [1, 2]. By obtaining numerical values for the angular momentum functions and taking into account all relevant symmetries, the explicit formulae for any observable quantity are computed for a given set of $(l, s, J)$-matrix elements.

*Restrictions on the complexity of the problem*

A set of 40 matrix elements can be accomodated, which should suffice for nearly all practical applications. The number of expansion coefficients is limited to 20 and only those vector addition coefficients which involve factorials of argument less than 31 can be computed. If these limits are exceeded unintentionally, a message is printed out.

*Typical running time*

Running time depends critically on the number of matrix elements, the complexity of the spin space involved and the type of observable calculated. Approximate running times for cross-sections involving vector and tensor polarized deuteron beams are for a set of 10 matrix elements: 1 min; for a set of 20 matrix elements: 2 min; for a set of 30 matrix elements: 4 min.

*Unusual features of the program*

As compared to TENMO [3], a similar program intended mainly for computational purposes, both ease of further computer applications and convenience in a direct use of the output for the analysis of nuclear reactions [4] have been stressed. Thus all relevant symmetry properties are taken into account and reflected by corresponding output. For each observable the appropriate formula is synthesized and printed out.

*References*

[1] T.A. Welton, Fast neutron physics; vol. II (Interscience, New York, 1963) chap. V, F.

[2] S. Devons and L.J.B. Goldfarb, Handbuch der Physik, Vol. 42 (1957) 362.

[3] R.D. McCulloch, H.W. Graben, S.T. Thornton and H.B. Willard, ORNL-Report 4121.

[4] F. Seiler and E. Baumgartner, Nucl. Phys. A153 (1970) 193.

COMPUTER PHYSICS COMMUNICATIONS 6 (1974) 240–242. NORTH-HOLLAND PUBLISHING COMPANY

# FIRST COLLISION GAMMA-RAY DOSE☆

Lincoln B. HUBBARD
*Furman University,*
*Greenville, South Carolina, USA*

Received 21 August 1973

## ADAPTATION SUMMARY

*Title of adaptation*: DOSEI IMPROVEMENTS

*Adaptation number*: 0001

*Catalogue number*: ACMG; *Title*: DOSEI; *Ref. in CPC*: 2(1971) 449

*Author of original program*: Lincoln B. Hubbard

*Computer*: IBM 360/65; *Installation*: Laboratory for Nuclear Science, Massachusetts Institute of Technology

*High speed store required*: 2100 words.

*No. of bits in a word*: 32

*No. of cards required to effect adaptation (including directive cards)*: 187

*Nature of changes*
This adaptation consists of three changes. Two of these speed execution. The other makes the results more accurate.

*Method of solution*
A geometric symmetry in the attenuation integral speeds execution. When reflectional or rotational symmetries exist in both source and matter distributions these can be utilized to speed execution. The attenuation in the source and target sub-volumes is added by three formulae adapted from spheres; two are in the literature and one is based on a point source.

*Restrictions on the complexity of the problem*
The attenuation will be calculated to within 2% provided the geometrical representation is good and the $x$, $y$, and $z$ spacings are equal and less than one mean free path.

*Typical running time*
Total execution time for the sample run required 1.2 min.

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☆ Research sponsored in part by the Research Corporation.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 13–37. NORTH-HOLLAND PUBLISHING COMPANY

# FORTRAN PROGRAM TO CALCULATE FINITE-RANGE NO-RECOIL DWBA TRANSFER CROSS SECTIONS

G.L. PAYNE and P.L. Von BEHREN
*Department of Physics and Astronomy, The University of Iowa,*
*Iowa City, Iowa 52242, USA*

Received 10 July 1973

## PROGRAM SUMMARY

*Title of program*: FINITE RANGE DWBA PHASE 1

*Catalogue number*: ABOW

*Computer*: IBM 360/65; *Installation*: University of Iowa Computer Center

*Operating system*: HASP OS/360

*Programming language used*: FORTRAN

*High speed storage required*: 24,576 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1539

*Keywords*: Nuclear, distorted-wave-Born-approximation, finite range, stripping, pick-up, transfer reactions

## PROGRAM SUMMARY

*Title of program*: FINITE RANGE DWBA PHASE 2

*Catalogue number*: ABOX

*Computer*: IBM 360/65; *Installation*: University of Iowa Computer Center

*Operating system*: HASP OS/360

*Programming language used*: FORTRAN

*High speed storage required*: 24,576 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1590

*Keywords*: Nuclear, distorted-wave-Born-approximation, finite range, stripping, pick-up, transfer reactions.

*Nature of physical problem*

The program calculates angular distributions produced by direct nuclear transfer reactions. In this type of reactions one assumes that a nucleon or cluster of nucleons is transferred directly from a bound state in the projectile nucleus to a bound state in the target nucleus.

*Method of solution*

The angular distributions are calculated by using the Distorted-Wave-Born-Approximation (DWBA) with the additional approximation of no-recoil.

The method used here is that of Sawaguri and Tobocman [1]. With this method one uses harmonic oscillator functions to expand the final bound-state wave function and to expand the initial bound-state wave function times its corresponding potential. These expansions are then used to generate a series expansion for the form factor or transfer function. This transfer function is then used to calculate the distorted partial-wave matrix elements which are used to generate the angular distribution.

Phase 1 calculates the form factor, or transfer function for each possible transferred $L$-value for given single-particle levels in both the initial and final bound states of the transferred particle. Other sets of single-particle levels may be included by running Phase 1 as many times as necessary. Phase 2 calculates the differential cross section by using the transfer function from Phase 1 to evaluate the matrix elements for each set of partial waves in the initial and final channels. Only the optical-model parameters are variable in Phase 2 since the contribution of the bound states to the matrix elements is fixed by Phase 1.

### *Restrictions on the complexity of the problem*

The restrictions due to the "no-recoil" approximation are discussed in the theory section of the Long Write-Up. The program is also restricted to interactions (in both bound-state and optical-model potentials) which have no spin dependence.

### *References*

[1] T. Sawaguri and W. Tobocman, J. Math. Phys. 8 (1967) 2223.

COMPUTER PHYSICS COMMUNICATION 7 (1974) 38–49. NORTH-HOLLAND PUBLISHING COMPANY

# ELECTRON IMPACT EXCITATION CROSS SECTIONS

M.R.C. McDOWELL☆, L. MORGAN★
*Royal Holloway College, Englefield Green, Surrey, UK*

and

V.P. MYERSCOUGH
*Applied Mathematics Dept., Queen Mary College,*
*Mile End Road, London, UK*

Received 25 September 1973

## PROGRAM SUMMARY

*Title of program*: POLORB

*Catalogue number*: AAGW

| *Computer*: | *Installation*: |
|---|---|
| CDC 7600 | NCAR, Boulder, Colorado |
| CDC 6600 | ULCC, University of London |
| ICL 1904S | Queen Mary College, London |

*Operating system*: SCOPE, MAXIMOP

*Programming language used*: FORTRAN IV

*High speed storage required*: 31 kwords

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1722

*Keywords*: Atomic, scattering, electron, hydrogen-like ion, distorted wave, Coulomb Born, Born Oppenheimer, excitation, S-states, Numerov.

*Nature of the physical problem*
Determines total and differential cross sections for the electron impact induced 1s → *n*s transitions in hydrogenic systems in a number of approximations. The main case is the DWPO model of [1].

*Method of solution*
A partial wave expansion is used. The radial scattering functions are obtained by a non-iterative method and normalized by matching to a JWKB solution.

*Restrictions on the complexity of the problem*
Only 1s → *n*s transitions are treated and without modification to COEFFS, $n \leqslant 5$. An extension to 1s → *n*p transitions is in preparation.

*Typical running time*
DWPO calculations take up to 60 sec CPU time on a CDC 6600, depending on the number of partial waves required for convergence. Born, Born–Oppenheimer, CB1 and CBO1 calculations require less than 5 sec per case.

*Reference*

[1] M.R.C. McDowell, L.A. Morgan and V.P. Myerscough, J. Phys. B (Atom and Molec. Phys.) 6 (1973) 1435.

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☆ Mathematics Department
★ Department of Statistics and Computer Science

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 50–62. NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAM FOR CALCULATING LEED INTENSITIES BASED ON THE INELASTIC COLLISION MODEL:
## I. MATRIX INVERSION METHOD

V. HOFFSTEIN☆

*Laboratoire de spectrométrie physique★,*
*B.P. 53 Centre de tri, 38041 Grenoble Cédex, France*

Received 24 May 1973

## PROGRAM SUMMARY

*Title of program*: ICMLEED – MATRIX INVERSION

*Catalogue number*: ACMK

*Computer*: IBM 360/67; *Installation*: Institute of Applied Mathematics Grenoble, France.

*Operating system*: OS 360/67

*Programming language used*: FORTRAN IV

*High speed storage required*: 43250 words.

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1909

*Keywords*: Solid state, LEED, low-energy electron diffraction, Debye model, $T$ matrix, inelastic collision model, lattice vibration, muffin-tin.

*Nature of physical problem*
The program calculates the intensities of electrons diffracted by crystal surfaces as a function of all incidence parameters.

*Method of solution*
The $T$ matrix method is used to treat multiple scattering and inelastic collisions.

*Restrictions on the complexity of the problem*
The program is restricted to the following cases: (1) Debye model for lattice vibrations. (2) Constant inelastic collision mean free path. (3) Phenomenological form of self-energy. (4) Muffin-tin model.

*Typical running time*
The time depends critically on several parameters, phase shift, number of recips used in expansions, etc. This version takes 36 sec per point.

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☆ Present address: School of Medicine, University of Miami, Biscayne Annex, Florida 33152, USA.

★ Laboratory associated to the "Centre National de la Recherche Scientifique".

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 73–84. NORTH-HOLLAND PUBLISHING COMPANY

# A NON-RELATIVISTIC SCF ATOMIC PROGRAM TO COMPUTE ONE-ELECTRON ENERGIES, TOTAL ENERGIES, AND SLATER INTEGRALS☆

John H. WOOD and Michael BORING

*University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, USA*

Received 9 April 1973

## PROGRAM SUMMARY

*Title of program*: HERSKLZARE

*Catalogue number*: AAKG

*Computer*: CDC 6600, CDC 7600. *Installation*: Los Alamos Scientific Laboratory

*Operating system*: SCOPE

*Programming language used*: FORTRAN IV

*High speed store required*: 34,176 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals are used*: Card reader, card punch, printer

*No. of cards in combined program and test deck*: 3445

*Keywords*: Atomic structure, self-consistent field, Herman–Skillman, Hartree–Fock–Slater.

*Nature of physical problem*

The program HERSKLZARE performs non-spin-polarized nonrelativistic self-consistent field calculations for atoms and ions through use of an approximate exchange potential (a number of different approximations are available to the program). Having calculated central field radial wave functions and eigenvalues, the total energy, *I*, *F*, *G* integrals, etc., can be calculated.

*Method of solution*

The differential equations are solved by the Numerov method. Self-consistency is obtained by interation. Integrals are calculated by Simpson's rule.

*Restrictions on complexity of the problem*

There is provision for 12 orbitals (*n*, *l*); this can easily be expanded.

*Unusual features in the program*

There is provision for using a number of different exchange potentials in the program. Hartree–Fock parameters can be calculated from the one-electron wave functions.

*Typical running time*

On the CDC 6600 a few seconds are required.

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☆ Work performed under the auspices of the U.S. Atomic Energy Commission.

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COMPUTER PHYSICS COMMUNICATION 7 (1974) 85–94. NORTH-HOLLAND PUBLISHING COMPANY

# DEPTH DISTRIBUTION OF ENERGY DEPOSITION BY ION BOMBARDMENT☆

Irwin MANNING and G.P. MUELLER★

*Nuclear Sciences Division, Naval Research Laboratory, Washington, D.C. 20375, USA*

Received 7 June 1973

## PROGRAM SUMMARY

*Title of program*: E-DEP-1

*Catalogue number*: ACIB

*Computer*: CDC-3800. *Installation*: Naval Research Laboratory

*Operating system*: SCOPE

*Programming languages used*: FORTRAN

*High speed store required*: 14,475 words.

*No. of bits in a word*: 48

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 2047

*Keywords descriptive of problem and method of solution*:
Nuclear, solid state, radiation damage, ion beams, heavy-ion beams, energy deposition, Johnson–Gibbons, Lindhard, LSS, ion ranges.

*Nature of physical problem*
The code E-DEP-1 calculates the distribution of energy deposited into elastic collisions for a beam of heavy ions coming to rest in an amorphous target material of up to six atomic components.

*Method of solution*
The calculation is based on the approximation of Kulcinski et al. [1] which estimates the energy straggling by relating it to the range straggling. The mean range and range straggling are obtained from the theory of Linhard et al. (LSS) [2] by using the code of Johnson and Gibbons [3], which is included in E-DEP-1 as a subroutine. The calculation of Kulcinski et al. is refined by using the Lindhard partition theory [4] to exclude the energy lost to inelastic (non damage-producing) processes.

The program E-DEP-1 is a self-contained package, designed to be easily and economically run by people with little or no prior computing experience. We tried to anticipate modifications users would need and segmented the code into subprograms designed to allow these changes to be made simply and with confidence. The results of E-DEP-1 are compared with those of other theories in a companion paper [5].

*Typical running times*
Exclusive of compilation time, the code takes approximately 30 sec to prepare tables of nuclear and electronic stopping rates, range straggling parameters, etc. The calculation of the deposited energy distribution takes roughly 12 sec per beam ion energy. These times are for the case of 9 MeV Fe ions incident on a Fe target. A multi-component target increases the 30 sec preparation time somewhat.

*References*

[1] G.L. Kulcinski, J.J. Laidler and D.G. Doran, Radiation Effects 7 (1971) 195.
[2] J. Lindhard, M. Scharff and H.E. Schiott, Danske Videnskab. Selskab 33 No. 14 (1963).
[3] W.S. Johnson, J.F. Gibbons, *Projected range statistics in semiconductors* (dist. by the Stanford University Bookstore, 1969).
[4] J. Linhard, V. Nielsen, M. Scharff and P.L. Thompson, Danske Vindenskab. Selskab 33, No. 10 (1963).
[5] I. Manning and G.P. Mueller, *Approximate calculation of the depth distribution of energy deposition in ion bombardment*, to be published.

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☆ This work was supported in part by the Office of Naval Research under Project Order PO-3-0039.

★ Presidential Intern in Science and Engineering.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 95–113. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR THE EXTRACTION OF RADIATIVE LIFETIMES FROM EXPERIMENTAL BEAM-FOIL INTENSITY DECAY DATA

D.J.G. IRWIN [☆] and A.E. LIVINGSTON

*Department of Physics, The University of Alberta, Edmonton, Alberta, Canada*

Received 22 November 1972

## PROGRAM SUMMARY

*Title of program*: HOMER

*Catalogue number*: AAED

*Computer*: IBM 360/67; *Installation*: University of Alberta

*Operating system*: Michigan Terminal System (MTS)

*Programming language used*: FORTRAN IV

*High speed storage required*: 16335 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, card punch

*No. of cards in combined program and test deck*: 2021

*Keywords*: Atomic, ion, life-time, excited state, beam-foil, decay curve, chi-square fit.

*Nature of physical problem*

The problem is to analyse experimental beam-foil intensity decay data into a sum of exponential terms, each with an amplitude and lifetime parameter. The most apt number of parameters and the optimum value of each is to be determined, together with estimates of standard deviation.

*Method of solution*

The minimum of chi-square is sought in an iterative procedure. Normal equations are obtained from a first order Taylor expansion of the multi-exponential fitting function, together with an auxiliary binomial expansion to first order. Non-convergence is impeded by two devices. A modified Marquardt method is built in as an option [1]. Initial estimates may be computed from the data. Rejection of extra-statistical data points may be allowed [2].

*Restrictions on the complexity of the problem*

The complexity of the fitting function is arbitrarily limited to, at most, a six-parameter fit in the form of a sum of three exponential terms. Provision is made for adjustment of the number of parameters during the computation so that a 6-, 5-, 4-, 3- or 2- parameter best fit may be obtained.

*Typical running time*

Typical running time is about 2 seconds on the IBM 360/67 with the G compiler for 25 data points and a six-parameter fitting function. This estimate does not include compilation of the program. It is recommended that a compiled version of the program be used in the interests of economy.

*References*

[1] N.R. Draper and H. Smith, *Applied regression analysis* (Wiley, New York, 1967) p. 272.

[2] E.M. Pugh and G.H. Winslow, *The analysis of physical measurements* (Addison-Wesley, Reading, Massachusetts, 1966) p. 108.

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[☆] Present address: Department of Physics, St. Francis Xavier University-Sydney Campus, Sydney, Nova Scotia, Canada.

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# ENERGY-LEVEL CALCULATIONS WITH THE EXTENDED AROVMI MODEL[☆]

S.M. ABECASIS[★] and F.R. FEMENIA[‡]

*Laboratorio de Radiaciones, IIAE, Departamento de Física, Facultad de Ciencias Exactas y Naturales,*
*Ciudad Universitaria, Pabellón 1 – Nuñez, Buenos Aires, Argentina*

Received 25 October 1973

## PROGRAM SUMMARY

*Title of program*: EXTARO

*Catalogue number*: ABMG

*Computer*: IBM 360/50; *Installation*: Centro Computación Facultad de Ingeniería, Universidad de Buenos Aires.

*Operating system*: OS/360

*Programming language used*: FORTRAN IV

*High speed storage required*: 34304 words.

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 639

*CPC Library subprograms used:*

| Catalogue number: | Title: | Ref. in CPC: |
|---|---|---|
| ABOE | ENERGY LEVELS IN DAVYDOV MODEL | 2 (1971) 33 |

*Keywords*: Nuclear, energy level, energy ratio, AROVMI model, extended AROVMI model, Bessel interpolation, Rosenbrock minimization method.

*Nature of the physical problem*

This program provides the theoretical values for the energy levels and ratios calculated with the extended AROVMI model [1] in terms of the parameters $\gamma_0$ and $\rho$ when the latter is allowed to be negative. Specially, it yields those values concerned with the $\alpha$, $\beta$ and $\alpha\beta$ solutions and obviously, those of the $\gamma$ solution too which correspond to the original AROVMI model [2].

*Method of solution*

The actual values of the model parameters are found by means of a minimization procedure based on Rosenbrock's method [3] in the version presented by Sheppey [4]. A Bessel formula is applied to interpolate the energy levels of the restricted asymmetric rotor [5]. The usual analytical reduction of the cubic equation is used to find its real roots.

*Restrictions on the complexity of the problem*

Computations are performed with the energy levels of the ground-state rotational and quasi-rotational band from $I = 2$ up to 20 (in steps of 2) and those of the gamma and quasi-gamma bands for $I = 2$ up to 10 (in steps of 1).

*Typical running time*

The compilation of the main program and the subroutines CUBICR and ROSEN and the function SOLUTI, together with the link-edition process with the subprograms BLOCK DATA and INTER from the library, plus the execution of the test run took 2 minutes and 33 seconds on the 360/50.

*References*

[1] S.M. Abecasis, Nucl. Phys. A123 (1973) 98.
[2] S.M. Abecasis and E.S. Hernández, Nucl. Phys. A180 (1972) 485.
[3] H.H. Rosenbrock, Comp. J. 3 (1960) 175.
[4] G.C. Sheppey, CERN Yellow Report 68-5, Data Handling Division (1968) p. 105.
[5] A.S. Davydov and G.F. Filippov, Nucl. Phys. 8 (1958) 237.

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[☆] Work done under the partial auspices of the Consejo Nacional de Investigaciones Cientificas y Técnicas.

[★] Member of the Scientific Research Career of the Consejo Nacional de Investigaciones Cientificas y Técnicas, Argentina.

[‡] Member of the Technical Personnel Career of the Consejo Nacional de Investigaciones Cientificas y Técnicas, Argentina.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 151–162. NORTH-HOLLAND PUBLISHING COMPANY

# A FLEXIBLE LEAST SQUARES ROUTINE FOR GENERAL MÖSSBAUER EFFECT SPECTRA FITTING

W. WILSON and L.J. SWARTZENDRUBER
*National Bureau of Standards, Washington, D.C. 20234, USA*

Received 24 October 1973

## PROGRAM SUMMARY

*Title of program*: FLEXIBLE MÖSSBAUER FIT ROUTINE

*Catalogue number*: ACML

*Computer*: UNIVAC 1108; *Installation*: National Bureau of Standards, Gaithersburg, Maryland

*Operating system*: EXEC 8

*Programming languages used*: FORTRAN IV

*High speed store required*: 40,000 words

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 2023

*Keywords*: Nuclear, solid state, Mössbauer effect, spectra, least squares fit, non-linear, linearization, iterative solution.

*Nature of physical problem*

A general program is presented to fit experimental Mössbauer data to theoretical functions. The program is designed to allow the theoretical function to be easily changed.

*Method of solution*

The technique of linearization and successive interation is used to obtain a least squares fit of a non-linear theoretical function to the experimental data.

*Restrictions to the complexity of the program*

The present version of the program is dimensioned so that the maximum number of independent parameters the fitting function may have is 100 and a maximum of 40 of these may be varied at one time. The maximum number of data points allowed is 500. Any of these restrictions may be removed by increasing the dimensions of the appropriate variables.

*Typical running time*

On the UNIVAC 1108 at the National Bureau of Standards the loading and assembly of the program takes about 15 sec. The execution time is highly dependent on the number of data points, the complexity of the fitting function, the accuracy of the initial estimates, and the number of partial derivatives which are evaluated numerically. In a trial run, in which reasonable estimates were used and 6 partial derivatives were evaluated numerically, a 15 parameter function was fit to 320 data points in approximately 11 sec. The bulk of the time is utilized in calculating partial derivatives numerically. If $m$ parameters are being varied in the fit, each of which calls for numerical evaluation of partial derivatives, the theoretical function subroutine is called $m+4$ times for each iteration. Since 3 iterations are usually sufficient, a good estimate of the required time is $3\tau_f(m+4)+\tau_c$, where $\tau_f$ is the amount of time to calculate the theoretical function once and $\tau_c$ is the time consumed in compilation and output.

*Unusual features of the program*

The fitting function may be changed simply by replacing the appropriate subroutine. Thus a library of often used functions may be constructed. Partial derivatives the respect to the various parameters may be fit only over the range of data in which it has significance. The option of which parameters are to be varied is left to the user so that constraints and interdependence of variables may be easily taken into account by building them into the fitting function subroutine.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 163–171. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAMMING PACKAGE FOR THE CALCULATION OF CROSS-SECTIONS AND PROBABILITIES FOR CHARGE-EXCHANGE PROCESSES

J. van den BOS
*Department of Computer Science, University of Nebraska, Lincoln, Nebraska 68508, USA*

Received 10 October 1973

## PROGRAM SUMMARY

*Title of program*: IPFVAIJ

*Catalogue number*: ACRP

*Computer*: IBM 360/65; *Installation*: University of Nebraska

*Operating system*: HASP/OS 360 MVT

*Programming language used*: FORTRAN

*High speed storage required*: 23000 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: 2 (cards or magnetic disk may be used instead)

*Other peripherals used*: Cardreader; lineprinter; magnetic disk (cards optional)

*No. of cards in combined program and test deck*: 1031

*Keywords*: Atomic, molecular, collisions, charge exchange, electron capture, interaction matrix elements, overlap matrix elements, double numerical quadrature.

## PROGRAM SUMMARY

*Title of program*: IPFDEQ

*Catalogue number*: ACRQ

*Computer*: IBM 360/65; *Installation*: University of Nebraska

*Operating system*: HASP/OS 360 MVT

*Programming language used*: FORTRAN

*High speed storage required*: 20000 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: 1 (optional)

*Other peripherals used*: Magnetic disk (cards or magnetic tape may be used instead); cardreader; lineprinter

*No. of cards in combined program and test deck*: 992

*CPL Library subprograms used*

| Catalogue number | Title | Ref. in CPC: |
|---|---|---|
| ACRP | IPFVAIJ | 7 (1974) 161 |

*Keywords*: Atomic, molecular, collisions, charge exchange, electron capture, impact parameter, differential equations, predictor-corrector

*Nature of the physical problem*
When two atomic or molecular species collide there is a finite probability that they exchange electrons. In this communication we describe a method that results in probabilities and cross-sections for the process in which one of the particles captures an electron from the other one. The method is restricted to relative kinetic energies appreciably larger than the energy deficit of the reaction.

*Method of solution*
A finite-state expansion of the total wave function involved, when substituted in the Schrödinger equations, gives rise to a system of coupled linear differential equations, under the assumption of a straight-line trajectory for the projectile. IPFVAIJ computes the interaction and overlap matrix elements for the two reactants involved, while IPFDEQ solves the coupled equations as a function of impact parameter and kinetic energy of the projectile using a predictor-corrector method.

*Restrictions on the complexity of the problem*
The package has no restrictions on the kind of atoms or molecules involved except that it can only solve the following combinations of electronic spectral states: $l_1 = 0, l_2 = 0; l_1 = 0, l_2 = 1; l_1 = 1, l_2 = 0$.

*Unusual features of the program*
IPFVAIJ inputs wave functions and potentials from an user-constructed direct-access data base. This data base may be emulated on magnetic tape. The program also allows for a test option in which the data are input from a card file.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 172–173. NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAM ACRL TO CALCULATE DIFFERENTIAL AND INTEGRAL CROSS SECTIONS ADAPTED TO RUN ON IBM COMPUTERS[☆]

Maynard A. BRANDT, Donald G. TRUHLAR and Richard L. SMITH[‡]
*Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455, USA*

Received 22 January 1974

## ADAPTATION SUMMARY

*Title of adaptation*: ACRL ADAPTED FOR IBM 360 OR 370

*Adaptation number*: 0001

*Reference to original program*:

| *Catalogue number*: | *Title*: | *Ref. in CPC*: |
|---|---|---|
| ACRL | DCS | 5 (1973) 456. |

*Authors of original program*: M.A. Brandt, D.G. Truhlar and R.L. Smith

| *Computer*: | *Installation*: |
|---|---|
| IBM 370/145 | Administrative Data Processing Division of Management Planning and Information Services of the University of Minnesota |
| CDC 6600 | University Computer Center of the University of Minnesota |

*Operating system*: OS/VS1 (IBM) or SCOPE 3.2 (CDC)

*High speed store required*: 17500 words (IBM).

*No. of bits in a word*: 32 (IBM).

*No. of cards required to effect adaptation (including directive cards)*: 27

*Typical running time*

The test run [1] required 142 sec (CPU time, excluding compilation and load time) on the IBM 370/145.

*Reference*

[1] M.A. Brandt, D.G. Truhlar and R.L. Smith, Computer Phys. Commun. 5 (1973) 456; 7 (1974) 177.

## ERRATUM

Maynard A. Brandt, Donald G. Truhlar, and Richard L. Smith, Program for calculating differential and integral cross sections for quantum mechanical scattering problems from reactance or transition matrices, Computer Physics Communications 5 (1973) 456.

In eq. (14) on p. 463 the $)^{\frac{1}{2}}$ should be $)]^{\frac{1}{2}}$. The first equation defining

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{pmatrix}$$

on p. 463 should be designated eq. (12/6.3.7). In the second line of subsection 3C) on p. 467, 4-state should be replaced by 2-state, 4-channel. The fourth line of table 2 on p. 467 should have the same JINDEX values as does the third line of table 2. Ref. [10] should be M.A. Brandt and D.G. Truhlar, Phys. Rev. A, to be published; D.G. Truhlar, C.A. Mead, and M.A. Brandt, Adv. Chem. Phys., to be published. The name of the first author of ref. [13] should read R.S. Caswell.

---

[☆] Research supported in part by the National Science Foundation under research grant no. GP-28684 and by the University Computer Center and the Graduate School of the University of Minnesota.

[‡] Present address: Amoco Production Company, Amoco Building, P.O. Box 50879, New Orleans, Louisiana 70150, U.S.A.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 185–191. NORTH-HOLLAND PUBLISHING COMPANY

# MONTE CARLO SIMULATION OF PHOTONS IN TWO–LAYERED MEDIA FOR DENSITY GAUGES

E.R. CHRISTENSEN

*Department of Electrophysics, The Technical University,*
*DK-2800 Lyngby, Denmark*

Received 22 November 1973

## PROGRAM SUMMARY

*Title of program*: MCS

*Catalogue number*: AAUK

*Computer*: IBM 370/165; *Installation*: Northern Europe University Computing Center, DK-2800 Lyngby, Denmark

*Operating system*: HASP-II

*Programming language used*: FORTRAN IV

*High speed store required*: 18498 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, card punch

*No. of cards in combined program and test deck*: 867

*Keywords*: Nuclear, photon scattering, Monte Carlo method, two-layered medium, density gauge, principle of similitude, axial symmetry.

*Nature of physical problem*
Multiple photon scattering in a two-layered medium is considered. The photons are assumed to originate from a mono-energetic point source situated at an arbitrary height over the medium. The relative number of backscattered photons, weighted with a detector efficiency spectrum, is calculated in consecutive radial intervals.

*Method of solution*
Photons are simulated by the Monte Carlo method [1]. Stratified sampling is applied to the isotropically emitted source photons. The scattering angle is determined by iteration from the Klein–Nishina cross section.

*Restrictions on the complexity of the problem*
A maximum of 12 elements, 19 energy groups, 16 radial-, and 18 depth intervals may be considered. The perpendicular to the plane medium, through the source, is an axis of symmetry, and thus only axial symmetrical problems can be solved.

*Typical running time*
Simulation of 90 000 photon histories takes about 3 min of central processor time.

*Unusual features of the program*
Responses in different radial intervals can by the principle of similitude be interpreted as responses in a given interval at different densities. This presupposes a source height of zero, a semi-infinite medium and similar radial intervals.

*Reference*

[1] Y.A. Schreider, ed., *The Monte Carlo method* (Pergamon, Oxford, 1966).

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 192–199. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTER SIMULATION OF PHOTONS IN SPHERIC MEDIA FOR DENSITY GAUGES

E.R. CHRISTENSEN
*Department of Electrophysics, The Technical University,*
*DK-2800 Lyngby, Denmark*

Received 14 December 1973

## PROGRAM SUMMARY

*Title of program*: MCD

*Catalogue number*: AAUL

*Computer*: IBM 370/165; *Installation*: Northern Europe University Computing Center, DK-2800 Lyngby, Denmark

*Operating system*: HASP-II

*Programming languages used*: FORTRAN IV

*High speed store required*: 23262 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 631

*CPC Library subprograms used*:

| *Catal. number*: | *Title*: | *Ref. in CPC*: |
|---|---|---|
| AAUK | MCS | 7 (1974) 185 |

*Keywords*: Nuclear, photon scattering, Monte Carlo method, spheric medium, density gauge, principle of similitude, least-squares fit.

*Nature of physical problem*
Multiple photon scattering in a spheric medium is considered. The photons are assumed to originate from a monoenergetic point source situated at the center. The relative photon track length, weighted with a detector efficiency spectrum, is calculated in consecutive radial intervals. In order to contribute to the track length, the elements of the photon paths must form an angle with radius vector which is greater than a specified cut-off angle.

*Method of solution*
Photons are simulated by the Monte Carlo method [1]. The scattering angle is determined by iteration from the Klein–Nishina cross section. A least-squares fit of an analytical expression to the calculated results is performed.

*Restrictions on the complexity of the problem*
A maximum of 12 elements, 19 energy groups, 50 radial-, and 11 importance intervals may be considered. The medium is spheric and homogeneous.

*Typical running time*
Simulation of 24 000 histories takes about 3 min of central processor time.

*Unusual features of the program*
Responses in different radial intervals can by the principle of similitude be interpreted as responses in a given interval at different densities. This presupposes an infinite medium and similar radial intervals.

*Reference*

[1] Y.A. Schreider, Ed., *The Monte Carlo method* (Pergamon, Oxford, 1966).

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 200–206. NORTH-HOLLAND PUBLISHING COMPANY

# INVERSION OF ABEL'S INTEGRAL EQUATION – APPLICATION TO PLASMA SPECTROSCOPY

C. FLEURIER and J. CHAPELLE
*Centre de Recherches sur la Physique des Hautes Températures,*
*CNRS, Orléans, France*

Received 3 October 1973

## PROGRAM SUMMARY

*Title of program*: ABEL

*Catalogue number*: AAAC

*Computer*: IBM 360/25; *Installation*: G.R.I. – CNRS – Orléans, France

*Operating system*: DOS/360

*Programming language used*: FORTRAN IV

*High speed store required*: 7373 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 433

*Keywords*: Plasma spectroscopy, Abel integral equation, least-squares approximation.

*Nature of the physical problem*

The purpose of this program is to determine the radial distribution of the emission coefficient from the measured intensity distribution emitted by an extended source of radiation, particularly a plasma source. The source is assumed to be optically thin and axially symmetrical.

*Method of solution*

This problem is solved by inverting Abel's integral equation [1]. A smoothing procedure is made on the experimental curve in order to attenuate the random errors before computing the derivative. The integral is calculated analytically in a small interval on the right of the discontinuity point, the other part is estimated numerically.

*Restrictions on the complexity of the problem*

The computation is nearly entirely numerical and needs equally spaced points for the data.

*Typical running time*

For an experimental curve defined by 21 points the calculation time is less than 30 s on the IBM 360/25 computer.

*Reference*

[1] R. Bracewell, *The Fourier transform and its applications* (Mac-Graw Hill, New York, 1965), p. 262–265.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 207–214. NORTH-HOLLAND PUBLISHING COMPANY

# CALCULATION OF CRYSTAL POTENTIALS

Dimitrios A. PAPACONSTANTOPOULOS

and

Wayne R. SLAUGHTER

*George Mason University, Fairfax, Virginia 22030, USA*

Received 6 June 1973

## PROGRAM SUMMARY

*Title of program*: CRYSTAL POTENTIALS

*Catalogue number*: ACID

| *Computer*: | *Installation*: |
|---|---|
| CDC 6400 | Computer Science Center, University of Virginia, Charlottesville, Virginia 22901, USA |
| CDC 3800 | Research Computer Center, Naval Research Laboratory, Washington, D.C. 20375, USA |
| IBM 360/50 | Computer Center, College of William and Mary, Williamsburg, Virginia 23185, USA |

*Operating system*: SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: 110,000 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: 2

*Other peripherals used*: Card reader, card punch, lineprinter

*No. of cards in combined program and test deck*: 2012

*Keywords*: Solid state, crystal potential, band structure, Löwdin α-expansion, cubic lattice, muffin-tin potential, fcc, bcc, NaCl, CsCl, Hartree–Fock–Slater.

*Nature of physical problem*
The program constructs crystal potential for band structure calculations.

*Method of solution*
A starting potential is constructed by a superposition of atomic charge densities by the Löwdin α-expansion and subsequent solution of Poisson's equation. A self-consistent potential is obtained by an iterative procedure in which the wave functions generated by an energy band calculation are used.

*Restrictions on the complexity of the problem*
The program is limited to cubic lattices.

*Typical running time*
1 Atom – 10 sec, 2 atoms – 25 sec.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 215–224. NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAMS FOR THE LANDAU AND THE VAVILOV DISTRIBUTIONS AND THE CORRESPONDING RANDOM NUMBERS

B. SCHORR
*Data Handling Division, CERN, Geneva, Switzerland*

Received 19 September 1973

## PROGRAM SUMMARY

*Title of program*: LANDAU

*Catalogue number*: AAUI

*Computer*: CDC 6600; *Installation*: CERN, Geneva

*Operating system*: CDC Scope

*Programming language used*: FORTRAN IV

*High speed storage required*: 1114 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 300

*Keywords*: Nuclear, Landau distribution, energy loss, thin absorber, random number generation.

## PROGRAM SUMMARY

*Title of program*: VAVILOV

*Catalogue number*: AAUJ

*Computer*: CDC 6600; *Installation*: CERN, Geneva

*Operating system*: CDC Scope

*Programming language used*: FORTRAN IV

*High speed storage required*: 3246 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, pine printer

*No. of cards in combined program and test deck*: 636

*Keywords*: Nuclear, Vavilov distribution, energy loss, thin absorber, random number generation.

*Nature of the physical problem*
The Landau [1] and the Vavilov [2] distributions are used to describe the energy loss of charged particles traversing a thin layer of matter. For Monte Carlo simulations it is of particular interest to have a random number generator for these distributions.

*Method of solution*
Fourier series are used to approximate the probability density functions, the cumulative distribution functions and the inverses of the conditional distribution functions.

*Restrictions on the complexity of the problem*
Theoretical considerations, together with numerical tests, show that in the case of the densities and the distribution functions three to five significant digits are obtained. In the case of the inverses of the conditional distribution functions three significant figures are obtained almost everywhere, except near the end points of the interval, where a relative error of up to 5–6% may occur.

*References*

[1] L. Landau, J. Phys. 8 (1944) 201–205.
[2] P.V. Vavilov, Zh. Exper. Teor. Fiz. 32 (1957) 920–923
[English transl. JETP 5 (1957) 749–751].

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 225–234. NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM TO EVALUATE THE REDUCED MATRIX ELEMENTS OF ONE-PARTICLE TENSOR OPERATORS FOR THE CONFIGURATIONS IN *JJ*-COUPLING

J.J. CHANG*

*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, BT7 1NN, Northern Ireland*

Received 16 December 1973

## PROGRAM SUMMARY

*Title of program*: RDMEJJ

*Catalogue number*: AAAD

| *Computer*: | *Installation*: |
|---|---|
| ICL 1906A | Atlas Computer Laboratory, Chilton, Didcot, Berks., UK |
| IBM 370/165 | CECAM, Bâtiment 506, 91-Campus d'Orsay, France |

*Operating system*: George 4

*Programming language used*: FORTRAN IV

*High speed storage required*: 20480 words

*No. of bits in a word*: 24

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1552

*CPC Library subprograms used*:

| *Catalogue number* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAGD | NJSYM | 1 (1970) 241,<br>2 (1971) 173 |
| AAGD0002 | ADAPT TO INTEGER ARITHMETIC | 5 (1973) 161 |
| ACRI | CFPJJ-CFP IN JJ-COUPLING | 4 (1972) 377 |

*Keywords*: Atomic, nuclear, transitions, electric multipole, magnetic multipole.

*Nature of the physical problem*
In relativistic atomic calculations and nuclear shell theory, many problems involve matrix elements of one-particle tensor operators, such as electric and magnetic multipole transitions. This program is designed to evaluate the angular part of these matrix elements between arbitrary configuration in *jj*-coupling.

*Method of solution*
Configurations are defined by the number of electrons and the $(n\kappa)$ quantum numbers in each occupied shell and coupling intermediate angular momenta. The angular integral of the reduced matrix element is expressed in terms of recoupling coefficients and coefficients of fractional parentage.

*Restrictions on the complexity of the program*
The program assumes that both configurations are formed from the same orthonormal set of basis orbitals. The number of electrons in orbitals with $j > \frac{9}{2}$ is restricted to be one or two by the available fractional parentage routines.

*Typical running time*
The time required for the test run is 71 sec of ICL 1907, of which 7 sec is taken in execution.

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* Present address: C.E.C.A.M., Bâtiment 506, Campus d'Orsay, 91, Orsay, France.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 236. NORTH-HOLLAND PUBLISHING COMPANY

# ERRATUM NOTICE

*Title of manuscript*: A multi-configuration Hartree–Fock program with improved stability.

*Author*: Charlotte Froese Fischer

*Reference*: Computer Phys. Commun. 4 (1972) 107

*Title of program*: MCHF72

*Catalogue number*: ACRF

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 245–270. © NORTH-HOLLAND PUBLISHING COMPANY

# OLYMPUS
# A STANDARD CONTROL AND UTILITY PACKAGE FOR INITIAL-VALUE FORTRAN PROGRAMS

J.P. CHRISTIANSEN and K.V. ROBERTS
*UKAEA Research Group, Culham Laboratory,*
*Abingdon, Berks., UK*

Received 10 December 1973

## PROGRAM SUMMARY

*Title of program:* OLYMPUS

*Catalogue number:* ABUF

*Computer:* ICL 4-70; *Installation:* UKAEA Culham Laboratory

*Operating system:* ICL Multijob

*Programming languages used:* STANDARD FORTRAN

*High speed store required* *: 14464 words;

*No. of bits in a word:* 32

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Line printer

*No. of cards in combined program and test deck:* 2425

*Keywords:* General purpose, control, utility, package, initial-value problems, simulation, computation, standard, framework, kernel.

*Nature of physical problem*
A standard methodology has been established for constructing, testing and operating Fortran programs which solve equations describing initial-value problems. Such programs inevitably have many similar administrative tasks to perform and can therefore be given a similar structure. By standardizing this structure and making it as independent as possible of the computer system one can speed up the construction of programs and also facilitate communication between programmers, users and different computational physics groups [1, 2]. OLYMPUS is a control and utility package which is used to support the development and operation of initial-value and other Fortran programs written at Culham, one of which, MEDUSA 1, is described in the following paper [3].

*Method of solution*
The OLYMPUS package consists of three parts:

1. A kernel called CRONUS which comprises a main program, a general-purpose control subroutine COTROL, and a number of other subroutines some of which are dummies.
2. A set of utility subprograms called CYCLOPS.
3. A set of test and demonstration subroutines and data files called MINOS, which are first used to establish the OLYMPUS package on a different computer system and later serve as skeletons or templates from which a 'real' program can be built up.

CRONUS itself is a 'null' program whose underlying structure together with that of MINOS is reflected in every 'real' program which uses the OLYMPUS methodology.

*Restrictions on the complexity of the problem*
The OLYMPUS package can be adapted to run with minor changes on any computer system for which a Standard Fortran [4]☆ compiler is provided. Library facilities should preferably be available so that the user need not handle the components of the package directly, and the availability of NAMELIST (not part of Standard Fortran) is helpful but not essential. The version presented here as Catalogue Number ABUF uses channel numbers and control cards applicable to the ICL 4/70 Multijob Operating System used at Culham, and intending users may find it more convenient to employ the version to be described in ref. [5] which has been adapted for an IBM 370/165, or that described in ref. [6] which has been adapted for a CDC 6500. Although specifically designed for initial-value problems, the OLYMPUS methodology has

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* For the MINOS test program.

☆ Previously known variously as ISO, ANSI, USASI or ASA Fortran.

been found to work well for many other types of computer application.

*Typical running time*

The time taken by the null program CRONUS to perform a single step is 1.11 seconds on the ICL 4/70 at Culham Laboratory. The two MINOS tests occupy 3.23 seconds and 3.64 seconds respectively. Negligible overheads are imposed on any real calculation.

*References*

[1] K.V. Roberts, Computer Phys. Commun. 7 (1974) 237.

[2] K.V. Roberts and J.P. Christiansen, to be published as a Culham Lab. Report.

[3] J.P. Christiansen, D.E.T.F. Ashby and K.V. Roberts, Computer Phys. Commun. 7 (1974) 271,

[4] 'Standard Fortran Programming Manual', Computer Standards Series, National Computing Centre Ltd., Manchester, England (1970).

[5] M.H. Hughes, P. Roberts and K.V. Roberts, Computer Phys. Commun., to be submitted for publication.

[6] M.H. Hughes, Computer Phys. Commun., to be submitted for publication.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 271–287. © NORTH-HOLLAND PUBLISHING COMPANY

# MEDUSA
# A ONE-DIMENSIONAL LASER FUSION CODE

J.P. CHRISTIANSEN, D.E.T.F. ASHBY and K.V. ROBERTS
*UKAEA Research Group, Culham Laboratory,*
*Abingdon, Berks., UK*

Received 10 December 1973

## PROGRAM SUMMARY

*Title of program:* MEDUSA 1

*Catalogue number:* ABUG

*Computer:* ICL 4-70; *Installation:* UKAEA Culham Laboratory

*Operating system:* ICL Multijob

*Programming languages used:* STANDARD FORTRAN

*High speed store required:* 45000 words.

*No. of bits in a word:* 32

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Line printer

*No. of cards in combined program and test deck:* 6316

*CPC Library subprograms used:*

| *Catalogue number:* | *Title:* | *Ref. in CPC:* |
|---|---|---|
| ABUF | OLYMPUS | 7 (1974) 245 |

*Keywords:* Plasma physics, fluid dynamics, fusion, lasers, one-dimensional, lagrangian, two-temperature, implicit.

*Nature of physical problem*
The feasibility of laser fusion as a method for generating controlled thermonuclear power has so far been mainly based on computer simulation [1, 2]. MEDUSA 1 has been written to investigate in one space dimension some of the hydrodynamic and plasma processes that take place in a small pellet which is irradiated by laser light. The physics and mathematics of the model are described in detail in [3].

*Method of solution*
The plasma is described by 4 main dependent variables $\rho$, $u$, $T_i$, $T_e$, which represent respectively the density, velocity and ion and electron temperatures. These are functions of the time $t$ and of a single space variable $r$ which can be chosen to correspond to slab, cylindrical or spherical geometry as required. Subsidiary variables represent the chemical composition of the plasma in terms of the fractions of the various ionic species that are present, the composition varying in space and time due to the thermonuclear reactions that occur. The Navier–Stokes equations are supplemented by separate heat conduction equations for the ion and electron temperatures and a variety of additional effects are included. A lagrangian difference mesh is employed, the integration scheme being explicit for the hydrodynamics, and implicit for the heat conduction equations using the Crank–Nicholson scheme and the Gauss elimination method. Several iterations are performed at each timestep in order to take into account the non-linear dependence of the physical coefficients on the density and temperatures and to ensure convergence.

*Restrictions on the complexity of the problem*
Version 1 of MEDUSA is intended to provide as simple a model of the laser fusion process as possible, and a number of physical phenomena and situations have therefore been omitted which may be included in later versions. Ad hoc sections of code can however be inserted at many points throughout the program in order to modify the working of the standard version for specific runs using the EXPERT facility [4–6]. MEDUSA 1 will accept any realistically programmed laser pulse and will describe the resulting plasma phenomena with an accuracy that depends on the mesh size as well as on the convergence criteria. The maximum permissible mesh size is determined by the size of core store of the computer employed.

*Typical running time*
Execution times depend on the mesh size and convergence

criteria. On the ICL 4/70 at Culham Laboratory, 1000 timesteps with a maximum of 5 iterations per timestep take 300 seconds for a mesh size of 40.

*Unusual features of the program*
MEDUSA 1 is written in Standard Fortran [7] except for the use of the NAMELIST facility, and is optimized for speed rather than memory requirements. Subsets of the physics can be employed if appropriate logical switches are set. The structure of the whole program is highly modular and uses the OLYMPUS control and utility package described in refs. [4–6]. The graphical output section which is part of the program at the Culham Laboratory has been excluded from the published version since it uses the GHOST Graphical Output System which is not generally available.

*References*

[1] J. Nuckolls, L. Wood, A. Thiessen and G. Zimmerman, Nature 239 (1972) 139.
[2] J.S. Clarke, H.N. Fisher and R.J. Mason, Phys. Rev. Lett. 30 (1973) 89.
[3] J.P. Christiansen, D.E.T.F. Ashby and K.V. Roberts, Culham Laboratory Report CLM-R 130, available from HMSO.
[4] J.P. Christiansen and K.V. Roberts, Computer Phys. Commun. 7 (1974) 245.
[5] K.V. Roberts and J.P. Christiansen, to be published as a Culham Laboratory Report, available from HMSO.
[6] K.V. Roberts, Computer Phys. Commun. 7 (1974) 237.
[7] *Standard Fortran programming manual,* Computer Standards Series, National Computer Centre Ltd., Manchester, England (1970).

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 289–317. NORTH-HOLLAND PUBLISHING COMPANY

# MONTE CARLO CALCULATION OF MULTIPLE SCATTERING EFFECTS IN THERMAL NEUTRON SCATTERING EXPERIMENTS*

J.R.D. COPLEY**
*Argonne National Laboratory,*
*Argonne, Illinois 60439, USA*

Received 5 July 1973

## PROGRAM SUMMARY

*Title of program*: SLOW NEUTRON MULTIPLE SCATTERING

*Catalogue number*: ACIC

*Computer*: IBM 370/195; *Installation*: Argonne National Laboratory

*Operating system*: OS/360, Release 21.7

*Programming language used*: FORTRAN IV

*High speed storage required*: 75000 words.

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, magnetic disk (up to three files)

*No. of cards in combined program and test deck*: 5576

*Keywords*: Solid state, multiple scattering, thermal neutron scattering, elastic coherent scattering, elastic incoherent scattering, inelastic scattering, Monte Carlo method, alpha–beta sampling scheme.

*Nature of physical problem*
In a thermal neutron scattering experiment, the measured cross section includes both single and multiple scattering events. The former can be obtained from the measurements by subtracting an estimate for the latter, which is generally a smoother function of scattering angle and energy and thus can be calculated using an approximate scattering function.

*Method of solution*
The program is adapted from that of Bischoff [1]. Given a scattering function the program tracks successive neutrons within the sample and/or sample container in a Monte Carlo fashion. At each scattering point, the response, within each time channel and for each detector, is calculated. A cut-off is imposed to avoid tracking neutrons indefinitely. Single and multiple scattering contributions for each time channel and for each angle, are separately accumulated.

*Typical running time*
Once the scattering function has been set up, the Monte Carlo loop takes 0.2 to 0.5 milliseconds per collision, per angle, per time channel. Typical running times for a complete problem are of order 1–10 min on the IBM 370/195. If elastic coherent scattering is to be calculated, the program may take considerably longer to obtain adequate statistics.

*Unusual features of the program*
The minimum high speed storage requirement is about 49000 words. If inelastic scattering is included, further high speed storage is required, the amount depending on how accurately the inelastic scattering functions are defined. In the present case an extra 26000 words are used to store these functions.

*Restrictions on the complexity of the problem*
The present program is limited to one geometry and to no more than eight scattering angles. The sample (and sample container) must be isotropic materials.

*References*

[1] F.G. Bischoff, Ph.D. Thesis, Rensselaer Polytechnic Institute (1970);
F.G. Bischoff, M.L. Yeater and W.E. Moore, Nucl. Sci. Eng. 48 (1972) 266.

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* Based on work performed under the auspices of the U.S. Atomic Energy Commission.

** Present address: Institut Max von Laue-Paul Langevin, B.P. 156, 38042 Grenoble Cédex, France

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# ADAPTATION OF A GENERAL PROGRAM TO CALCULATE ANGULAR MOMENTUM INTEGRALS IN ATOMIC STRUCTURE: INCLUSION OF THE ONE-ELECTRON PART OF THE HAMILTONIAN

A. HIBBERT

*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, N. Ireland*

Received 5 February 1974

## ADAPTATION SUMMARY

*Title of adaptation*: ADAPT WEIGHTS FOR ONE-ELECT

*Adaptation number*: 0001

*Reference to original program*:

| *Catal. number:* | *Title:* | *Ref. in CPC:* |
|---|---|---|
| ACQV | WEIGHTS NEW VERSION | 2 (1971) 180. |

*Authors of original program*: A. Hibbert

*Computer*: ICL 1906A; *Installation*: Atlas Computer Laboratory. Chilton, Didcot, Berkshire, U.K.

*Operating system or monitor under which the program is executed*: George 3

*Programming language used in adapted program*: FORTRAN IV

*High speed store required*: 29 k words.

*No. of bits in a word*: 24

*No. of cards required to effect adaptation (including directive cards)*: 469

*CPC Library subprograms used*:

| *Catal. numbers:* | *Titles:* | *Refs. in CPC:* |
|---|---|---|
| ACQB | P SHELL C.F.P. | 1 (1969) 15 |
| ACRN | A NEW D SHELL CFP | 6 (1973) 88 |
| AAGD | NJSYM | 1 (1970) 241 |
| AAGD0001 | ADAPT NJSYM WEIGHTS | 2 (1971) 180 |
| AAGD0002 | ADAPT TO INTEGER ARITHMETIC | 5 (1973) 161 |

*Additional keywords*: One-electron operators

*Nature of physical problem*
The adaptation allows the matrix elements of the full Hamiltonian to be expressed as weighted sums of radial integrals.

*Method of solution*
The coefficients of these integrals are expressed in terms of fractional parentage coefficients and recoupling coefficients, using the techniques of Racah algebra.

*Typical running time*
The test run took 27 seconds on the ICL 1906A. The two-electron part alone took 111 seconds on an ICL 1907. Since the former machine is 4–5 times faster than the latter, the additional one-electron part takes only a small proportion of the overall time.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 327–342. NORTH-HOLLAND PUBLISHING COMPANY

# MONTE CARLO PROGRAMS FOR CALCULATING THREE-DIMENSIONAL HIGH-ENERGY (50 MeV–500 GeV) HADRON CASCADES IN MATTER

J. RANFT[☆] and J.T. ROUTTI[★]
*CERN, Geneva, Switzerland*

Received 10 September 1973

## PROGRAM SUMMARY

*Title of program*: FLUKA

*Catalogue number*: AAUH

*Computer*: CDC 6500, CDC 6600, CDC 7600; *Installation*: CERN, Geneva

*Operating system*: SCOPE 20

*Programming language used*: FORTRAN

*High speed storage required*: 40,000 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader and line-printer

*No. of cards in combined and test deck*: 1975

*Keywords*: Nuclear, high energy, Monte Carlo, high-energy reactions, transport theory, radiation doses.

## ADAPTATION SUMMARY

*Title of adaptation*: TRANKA FOR DEEP PENETRATION

*Adaptation number*: 0001

*Reference to original program*:

| *Catal. number*: | *Title*: | *Ref. in CPC*: |
|---|---|---|
| AAUH | FLUKA | 7 (1974) this paper |

*Authors of original program*: J. Ranft and J.T. Routti

*High speed store required*: 50,000 words

*No. of bits in a word*: 60

*No. of cards required to effect adaptation (including directive cards)*: 1292

*Nature of physical problem*
High-energy protons incident on a target or a block of material initiate hadron cascades which transport and deposit the energy of the interacting particles in matter. The resulting distributions of star densities and energy deposition are of interest in the analysis of accelerator radiation problems, background estimation for high-energy physics experiments, total absorption detectors, cosmic-ray transport, shielding for space vehicles, and activation of material in space.

*Method of solution*
Monte Carlo simulation with particle splitting and variance reduction methods are used. Protons, neutrons and charged and neutral pions are considered, and empirical production formulae are used.

*Restriction on the complexity of the problem*
Cylindrical geometries and homogeneous material are considered in programs FLUKA and TRANKA. Other geometries can be considered in separate programs.

*Typical running time*
A simulation of the core of the hadron cascade with program FLUKA typically requires some 15,000 histories corresponding to about 30 sec of central processor time on a CDC 7600 computer. About three times as many histories, and CPU time, are recommended for deep penetration problems analysed with program TRANKA.

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[☆] Visitor from Sektion Physik, Karl Marx Universität, Leipzig, GDR.

[★] Visitor from Helsinki University of Technology, Otaniemi, Finland.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 343. © NORTH-HOLLAND PUBLISHING COMPANY

# A VERSION OF A NUCLEAR OPTICAL MODEL CODE FOR SMALL COMPUTERS DESIGNED TO RUN ON A PDP-15

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*Department of Physics, Kansas State University, Manhattan, Kansas 66506, USA*

Received 1 Feburary 1974

## PROGRAM SUMMARY

*Title of program*: OPTIX KSU 1

*Catalogue number*: ACRR

*Computer*: PDP-15; *Installation*: Department of Physics, Kansas State University, Manhattan, Kansas, USA.

*Operating system*: BF

*Programming language used*: Fortran IV

*High speed storage required*: 14K words

*No. of bits in a word*: 18 for integer variable. 2 words per floating-point variable.

*Overlay structure*: Overlaid

*No. of magnetic tapes required*: 2 PDP DEC tapes

*Other peripherals used*: Lineprinter, typewriter, storage oscilloscope images

*No. of card images in combined program and test deck*: 3660

*Reference to other published version of this program*:

| *Catalogue no.*: | *Title*: | *Ref. in CPC*: |
|---|---|---|
| ABOU | OPTICS | 5 (1973) 69 |

*Keywords*: Nuclear, optical model, potential, heavy ion, elastic scattering, Schrödinger equation, spin-zero, spin-half, spin-one, spin-orbit, Fox–Goodwin, Coulomb, compound-elastic, scattering amplitudes, phase shifts, transmission coefficients, angular distributions, cross sections, vector polarization analysing power, tensor polarization analysing power.

*Nature of physical problem*

This is a version of the program OPTICS [1] which has been modified to run on the PDP-15 computer. Details of the program are given in ref. [1].

*Restrictions on the complexity of the problem*

These are the same as in ref. [1], except that the maximum number of L-values has been increased to 80 and the maximum number of radial mesh points has been increased to 400.

*Typical running time*

As in OPTICS [1] with $T_c = 200$ for the computer multiply time in μsec for an operating system using software for multiplication.

*Unusual features of the program*

The program is designed for PDP-15 computers with DECtape input. This program is available from the CPC Program Library in card image form on DECtape only.

*Reference*

[1] R.J. Eastgate, W.J. Thompson and R.A. Hardekopf, Computer Phys. Commun. 5 (1973) 69.

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† Permanent address: Department of Physics and Astronomy, University of North Carolina, Chapel Hill, North Carolina 27514, USA.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 344–352. © NORTH-HOLLAND PUBLISHING COMPANY

# A PROGRAM FOR THE ANALYTIC SIMULATION OF EXTENSIVE AIR SHOWERS

L. GOOREVICH
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*Sydney, 2006, Australia*

Received 19 November 1973

## PROGRAM SUMMARY

*Title of program*: CASCADE

*Catalogue number*: AAYF

*Computer*: CDC 6600; *Installation*: Terminal at University of Sydney

*Operating system*: Scope

*Programming language used*: FORTRAN IV

*High speed storage required*: 28K words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 940

*Keywords*: Astrophysics, nuclear, high energy, cosmic rays, extensive air showers, simulation, hadrons, nuclear cascade.

*Nature of physical problem*
Air shower simulations allow one to compare the predictions of various models with experimental results of extensive air showers (EAS) arrays. Direct Monte Carlo methods are not practical, in terms of computing time, for the ultra-high primary energy (~ $10^{20}$ eV) and low thresholds (~ 1 GeV) now detectable. An analytic method [1] is therefore used to predict the mean values of observables such as hadron energy spectra, muon shower size and electron shower size.

*Method of solution*
The diffusion equations for nucleons and charged pions are solved by the method of 'successive generations'. This involves an iterative procedure in which the energy spectra of nucleons and charged pions, as a function of depth, are found by numerical integration. Other observables are derived from these basic spectra [2].

*Restrictions on the complexity of the problem*
Fluctuations in the characteristics of particle interactions are not taken into account. Cascade development is assumed to be in one dimension. Production of K-mesons is not considered. The electron component secondary to the muons is not considered.

*Typical running time*
This depends on the required accuracy of integration but is typically about 1.5 minutes for one set of parameters.

*Unusual features of the program*
The particle production spectra include delta-function components representing the decay products of isobars.

*References*

[1] A. Ueda and N. Ogita, Prog. Theor. Phys. 18 (1957) 269.
[2] L. Goorevich and L.S. Peak, Proc. of the 13th Int. Conf. Cosmic Rays, Denver, 029, 030 (1973).

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COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 369–388. © NORTH-HOLLAND PUBLISHING COMPANY

# LEED INTENSITY CURVES BY THE LAYER-BY-LAYER METHOD AND PERTURBATION CALCULATION

J. RUNDGREN and A. SALWÉN

*Department of Theoretical Physics, Royal Institute of Technology, S-10044 Stockholm 70, Sweden*

Received 20 August 1973

## PROGRAM SUMMARY

*Title of program*: LEED BY LAYERS AND PERTURBATION

*Catalogue number*: ACKE

*Computer*: IBM 360/75; *Installation*: Royal Institute of Technology, Stockholm

*Operating system*: GUTS

*Programming language used*: FORTRAN

*High speed storage required*: 98 kwords

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1550

*Keywords*: Solid state, low energy electron diffraction, LEED, surface structure, adsorbed layers, electron scattering, layer-by-layer method, perturbation calculation, structure constants, lattice sums, muffin-tin.

*Nature of the physical problem*

Experiments with low energy electron diffraction (LEED) are used for investigating the structure of the surface regions of pure crystals and of crystals covered with an adsorbate. The diffraction pattern is observed and the intensities of the diffracted beams are recorded as functions of energy and direction of the incident electrons [1]. In order to find the composition of the unit mesh of the surface structure, a model is proposed for the lattice of the substrate plus overlayer, and LEED intensity curv are calculated. A LEED intensity program is presented in this work.

*Method of solution*

It is supposed that the surface structure can be sliced into well separated atomic layers, the two-dimensional lattices of which contain one atom per unit cell. The multiple scattering of the electrons by the sliced structure is calculated by means of the layer-by-layer method [2]. The periodic Green's function of a layer is calculated using direct lattice summation. The fluxes of the beams reflected by a series of layers are calculated with the aid of the perturbation method for renormalized forward scattering [3].

The program is based on the muffin-tin approximation to the periodic potential of the surface region. The phase shifts representing the scattering of the low energy electrons by the muffin-tins are required as input to the program.

*Restrictions on the complexity of the problem*

The program can take at most 5 phase shifts and 21 beams.

*Typical running time*

The intensity of a diffraction pattern corresponding to a single energy and direction of incidence takes 3.4 sec, when the number of beams is fixed at 21 and the accuracy of beam intensity is 0.001. If the number of beams is adjusted by the program against the energy, intensity versus energy-curves are calculated more economically. Under these circumstances patterns calculated at equal intervals between 20 and 100 eV take on the average 1.7 sec/pattern.

*References*

[1] P.J. Estrup and E.G. McRae, Surface Sci. 25 (1971) 1.
[2] J.L. Beeby, J. Phys. C 1 (1968) 82.
[3] J.B. Pendry, J. Phys. C 4 (1971) 3095.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 389–391. NORTH-HOLLAND PUBLISHING COMPANY

# FORM FACTOR PROGRAM FOR RAYLEIGH SCATTERING OF GAMMA RAYS BY BOUND ELECTRONS

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*II. Physikalisches Institut der Universität,*
*D-3400 Göttingen, West Germany*

Received 16 May 1974

## PROGRAM SUMMARY

*Title of program*: RAYLEIGH FORM FACTORS

*Catalogue number*: AAGY

*Computer*: UNIVAC 1108; *Installation*: GWDG Göttingen

*Operating system*: EXEC 8

*Programming language used*: FORTRAN IV

*High speed storage required*: 9000 words

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, printer

*No. of cards in combined program and test deck*: 306

*Keywords*: Atomic, gamma ray scattering, Rayleigh scattering, form factor, Dirac wave function.

*Nature of physical problem*
The program performs calculations of the form factors and corrected form factors for the elastic scattering of gamma rays by the electrons of a complete subshell of an atom on the basis of Dirac one-electron wave functions [1–3].

*Method of solution*
Closed-form expressions for the form factors and corrected form factors derived in ref. [3] are used.

*Restrictions on the complexity of the problem*
None.

*Typical running time*
On the UNIVAC 1108 computer, a few seconds are required.

*Unusual features of the program*
To include the effects of screening the atomic number $Z$ and the electron energy eigenvalue may be modified.

*References*

[1] M. Schumacher, F. Smend and I. Borchert, Nuclear Phys. A206 (1973) 531.
[2] F. Smend, M. Schumacher and I. Borchert, Nuclear Phys. A213 (1973) 309.
[3] F. Smend and M. Schumacher, Nuclear Phys. A223 (1974) 423.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 392–400. NORTH-HOLLAND PUBLISHING COMPANY 392–400.

# NUCLEAR ENERGY LOSS AND SCATTERING OF IONS PENETRATING THIN LAYERS OF MATTER

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*Department of Physics, Chalmers University of Technology,*
*S-402 20 Göteborg, Sweden*

Received 24 April 1974

## PROGRAM SUMMARY

*Title of program*: NELAS

*Catalogue number*: AAUM

*Computer*: IBM 360/65; *Installation*: Gothenburg Universities Computing Centre

*Operating system*: OS/360 MFT II, HASP

*Programming language used*: FORTRAN

*High speed storage required*: 80,883 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: 1

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 711

*Keywords*: Nuclear, energy loss, scattering, distribution, thin layer, Monte Carlo method.

*Nature of the physical problem*
NELAS calculates the nuclear (elastic) energy losses and scattering distributions of initially monoenergetic and perfectly collimated ions penetrating a thin layer of matter.

*Method of solution*
The distributions are obtained by Monte Carlo simulation [1] using the reduced differential cross section in the form given by Lindhard and coworkers [2].

*Restrictions on the complexity of the problem*
The only assumptions made for the energy loss part of the calculation is that the collisions are perfectly elastic.

The low energy and large thickness limits are determined by the restriction that the energy loss should be much smaller than the mean energy of the ions. The target has to be amorphous or very fine polycrystalline.

*Typical running time*
Typical compile and running time is 70 seconds for step B, and 31 seconds plus 42 seconds for every 1000 ions run, when simulating a 4.0 $\mu$g/cm$^2$ (180 Å) carbon layer in step A.

*References*

[1] R. Skoog and G. Högberg, Rad. Effects
[2] J. Lindhard, V. Nielsen and M. Scharff, Mat. Fys. Medd. Dan. Vid. Selsk. 36, no. 10 (1968).

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 401–409. © NORTH-HOLLAND PUBLISHING COMPANY

# POSITRONFIT EXTENDED: A NEW VERSION OF A PROGRAM FOR ANALYSING POSITRON LIFETIME SPECTRA

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*Computer Installation, Danish Atomic Energy Commission, Research Establishment Risø,*
*DK-4000 Roskilde, Denmark*

and

Morten ELDRUP
*Chemistry Department, Danish Atomic Energy Commission, Research Establishment Risø,*
*DK-4000 Roskilde, Denmark*

Received 16 May 1974

## PROGRAM SUMMARY

*Title of program*: POSITRONFIT EXTENDED

*Catalogue number*: AAGX

| *Computer*: | *Installation*: |
|---|---|
| B 6700 | RISØ, Denmark |
| IBM 370/165* | NEUCC, Denmark |

*Operating system*: B6700 MCP Mark. II.6

*Programming language used*: Fortran

*High speed storage required*: 21000 words

*No. of bits in a word*: 48

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, lineprinter

*No. of cards in combined program and test deck*: 1222

*Reference to other published version of this program*:
*Catalogue number*: AAGK; *Title*: POSITRONFIT;
*Ref. in CPC*: 3 (1972) 240.

*Keywords*: Atomic, nuclear, positron, lifetime, time spectrum, source correction, least squares, fitting, convolution, minimization, sum-of-exponentials, iterations, Marquardt, constraints, covariance matrix.

*Nature of the physical problem*
Analysis of positron lifetime spectra, cf. description of the original version of POSITRONFIT [1].

*Method of solution*
Least-squares technique [1].

*Restrictions on the complexity of the program*
Maximal seven gaussian components in the resolution curve. Other restrictions as in [1].

*Typical running time*
The analysis of a single, typical lifetime spectrum takes about 85 sec on the B 6700 (or about 12 sec on the IBM 370/165).

*Reference*

[1] P. Kirkegaard and M. Eldrup, Computer Phys. Commun. 3 (1972) 240–55.

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* With minor changes.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 410–418. © NORTH-HOLLAND PUBLISHING COMPANY

# CALCULATION OF THE EQUILIBRIUM STRUCTURE AND OSCILLATIONS OF POLYTROPIC STARS PERVADED BY TOROIDAL MAGNETIC FIELDS

M.J. MIKETINAC

*Department of Applied Mathematics, University of Cape Town, Rondebosch, C.P., South Africa*

Received 17 December 1973

## PROGRAM SUMMARY

*Title of program*: TOROID

*Catalogue number*: AAAE

*Computer*: UNIVAC 1106; *Installation*: Computer Centre, University of Cape Town

*Operating system*: Exec 8

*Programming language used*: Fortran V

*High speed storage required*: 43K words.

*No. of bits in a word*: 36

*Overlay structure*: Overlaid

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1652

*Keywords*: Astrophysics, polytropic star, equilibrium configuration, toroidal magnetic field, frequencies of oscillation

*Nature of physical problem*

This program solves the structure equations determining the equilibrium configurations of a self-gravitating, axisymmetric, perfectly conducting polytrope with the polytropic index $n$ ($\geq 1$) in the presence of a toroidal magnetic field [1]. Parameters such as mass, volume, radius etc., characterising an equilibrium configuration are calculated. In addition, frequencies of the characteristic modes of oscillation are determined using Chandrasekhar's virial tensor method and assuming that the ratio of the specific heats, $\gamma$, is equal to 5/3.

*Method of solution*

The structure problem is mathematically a boundary-value problem for a second-order, non-linear, two-dimensional partial differential equation. This problem is solved numerically by following Stoeckly's method [2] improved by Miketinac and Barton [3], who used it to calculate post-newtonian corrections to the equilibrium configurations of rotating polytropes.

*Restrictions on the complexity of the problem*

The mathematical method adopted in developing the program works only for polytropes whose polytropic index is greater than or equal to one, [2]. However, in addition to calculating equilibrium configurations of polytropes pervaded by toroidal magnetic fields, the program, with minor modifications, could also be used for calculating equilibrium configurations of (uniformly or non-uniformly) rotating polytropes or rotating polytropes pervaded by toroidal magnetic fields or (rotating) polytropes containing toroidal magnetic fields of the type other than the one considered in [1]. The ratio of the specific heats, $\gamma$, can be any number.

*Typical running time*

The time required for the test run is 2 min and 54 sec on a UNIVAC 1106 computer, of which 5.16 sec is taken in compiling.

*References*

[1] M.J. Miketinac, Astrophys. Sp. Sci. 22 (1973) 413.
[2] R. Stoeckly, Astrophys. J. 142 (1967) 208.
[3] M.J. Miketinac and R.J. Barton, Astrophys. Sp. Sci. 18 (1972) 437.

COMPUTER PHYSICS COMMUNICATIONS 7 (1974) 419–427. © NORTH-HOLLAND PUBLISHING COMPANY

# PROGRAM FOR CALCULATING WORK FUNCTIONS FROM PHOTOELECTRIC DATA

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*Department of Pure and Applied Physics, The Queen's University of Belfast,*
*Belfast BT7 1NN, Northern Ireland*

Received 22 November 1973
Revised manuscript received 9 April 1974

## PROGRAM SUMMARY

*Title of program:* WORK

*Catalogue number:* ACKF

*Computer:* ICL 1906S; *Installation:* Queen's University of Belfast

*Operating system:* FLAIR

*Programming language used:* FORTRAN IV

*High speed storage required:* 2997 words

*No. of bits in a word:* 24

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer

*No. of cards in combined program and test deck:* 238

*Keywords:* Solid state, work function, photoelectric emission, Fowler plot, surfaces, method of bisection, least squares, error matrix.

*Nature of physical problem*
The work function of a metal may be obtained by fitting measurements of the photoelectric yield at various photon energies near the threshold to the theoretical Fowler curve [1]. The program carries out this curve-fitting operation.

*Method of solution*
A similar method of calculation has been described by Lea et al. [2]. The best fit is obtained by minimising the squares of the deviations between the experimental and theoretical ordinate values. The solution of the two normal equations resulting from this operation is by the method of bisection.

*Typical running time*
The execution time per curve fit is negligible (less than 1s). In practice, the number of curve fits is limited to the allowed number of lines output on the line printer (about 35 lines per fit).

*References*

[1] R.H. Fowler, Phys. Rev. 38 (1931) 45.
[2] C. Lea, B.H. Blott and C.H.B. Mee, Appl. Optics 8 (1969) 203.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 35–48. NORTH-HOLLAND PUBLISHING COMPANY

# QUANTUM MECHANICAL COUPLED CHANNELS CODE FOR COULOMB EXCITATION*

F. RÖSEL[☆] and J.X. SALADIN
*University of Pittsburgh, Pittsburgh, Pennsylvania 15213, USA*

and

K. ALDER
*University of Basel, Petersplatz 1, 4051 Basel, Switzerland*

Received 18 December 1973

## PROGRAM SUMMARY

*Title of program*: AROSA-FOR-COULOMB-EXCITATION-I

*Catalogue number*: ABOY

| *Computer*: | *Installation*: |
|---|---|
| PDP 1077 | University of Pittsburgh, USA |
| UNIVAC 1108 | Sandoz Co. Basel, Switzerland |

*Operating system*: FORSE (32A)

*Programming language used*: Fortran IV

*High speed storage required*: 39K words.

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: Optional in lieu of disc

*Other peripherals used*: Disc, card reader, line printer, card punch optional

*No. of cards in combined program and test deck*: 1686

*CPC Library subprograms used*:
*Catalogue number*: ABOZ; *Title*: AROSA-FOR-COULOMB-EXCITATION-II; *Ref in CPC*: 8 (1974) this paper.

*Keywords*: Nuclear, coupled channels, Coulomb-excitation, excitation amplitudes, excitation cross-sections, Schrödinger equation.

## PROGRAM SUMMARY

*Title of program*: AROSA-FOR-COULOMB-EXCITATION-II

*Catalogue number*: ABOZ

| *Computer*: | *Installation*: |
|---|---|
| PDP 1077 | University of Pittsburgh, USA |
| UNIVAC 1108 | Sandoz Co. Basel, Switzerland |

*Operating system*: FORSE (32A)

*Programming language used*: Fortran IV

*High speed storage required*: 39K words.

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: Optional in lieu of disc

*Other peripherals used*: Disc, card reader, line printer

*No. of cards in combined program and test deck*: 751

*CPC Library subprograms used*:
*Catalogue number*: ABOY; *Title*; AROSA-FOR-COULOMB-EXCITATION-I; *Ref. in CPC*: 8 (1974) this paper.

*Keywords*: Nuclear, coupled channels, Coulomb-excitation, excitation amplitudes, excitation cross-sections, Schrödinger equation.

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[*] Work supported by the National Science Foundation and the Swiss National Science Foundation.

[☆] Present address: Physics Department, University of Basel, Basel, Switzerland.

*Nature of physical problem*

AROSA calculates amplitudes and cross sections for Coulomb excitation of even even nuclei (g.s. spin and parity $0^+$). Up to five excited states may be included in the calculation. All reduced E2 and E4 matrix elements between these states may be taken into account.

*Method of solution*

The set of radial second-order differential equations resulting from the Schrödinger equation is solved by outward integration from the vicinity of the origin. The integration method is based on the Taylor expansion whose coefficients are obtained from recursion relations. At larger distances a WKB procedure is employed. Convergence of the scattering amplitudes with the number of partial waves is improved by using a procedure which is related to the Padé approximation.

*Restrictions on the complexity of the problem*

The Sommerfeld parameter $\eta$ must be smaller than 30, but methods are discussed for extrapolation of results to larger $\eta$ values.

*Typical running time*

The running time is roughly proportional to the square of the number $N$ of couplings which is given by $N = \Sigma_n(I_n + 1)$ where $I_n$ is the spin of the $n$th state. A calculation involving three states with spins and parities $0^+$, $2^+$, $4^+$ and all by selection rules permissible E2 and E4 matrix elements between them, requires on the PDP 1077 about 35 minutes.

*Unusual features*

Due to the long-range nature of the Coulomb force it is necessary to carry out the integration of the radial equations to large distances, and to assure convergence as a function of orbital angular momentum. The integration can be carried out to arguments $\rho = kr = 800$ and the convergence as a function of $l$ is improved by the use of an iterative procedure related to the Padé approximation.

The program can be executed in two parts with part I supplying data on cards for part II. Alternatively, the two sections can be run consecutively with intermediate data stored on disc.

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# SEARCH PROGRAM FOR SIGNIFICANT VARIABLES

M.J. O'CONNELL
*Rutherford High Energy Laboratory,*
*Chilton, Didcot, Berkshire, UK*

Received 4 February 1974

## PROGRAM SUMMARY

*Title of program:* LINCOM

*Catalogue number:* ABCG

| *Computer:* | *Installation:* |
|---|---|
| IBM 360/195 | RHEL, Chilton |
| ICL 1906A | Atlas Laboratory, Chilton |
| CDC6600 | CERN |

*Operating system:* IBM/OS with HASP

*Programming language used:* FORTRAN

*High speed store required:* 13K words

*No. of bits in a word:* 32

*Overlay structure:* None

*No. of magnetic tapes required:* 2

*Other peripherals used:* Card reader, line-printer

*No. of cards in combined program and test deck:* 964

*Keywords:* General purpose, nuclear high energy, significance search, dispersion matrix, significant variables, eigenvalues, eigenvectors.

*Nature of physical problem*
The coordinates associated with readings of one or more independent variables are converted into significant linear combinations of the original independent variables.

*Method of solution*
Eigenvalues and eigenvectors of the 'dispersion' matrix for the problem are calculated, and the 'position-vector' of each observation is analysed into the components along the normalized eigenvectors. If the eigenvalues are arranged in decreasing order or the linear combination in corresponding order, the most important linear combination is the first and the least important is the last. If some eigenvalues are very small relative to the largest, then the corresponding linear combination may be ignored or set to zero. In this way the complexity of a problem can be reduced. The derivation of momenta from spark chamber coordinates using this method has been discussed by Wind [1], from whose original program the present version has been standardised.

*Typical running time*
5 seconds on IBM 360/195 (including 2.6 seconds to compile) for analysis of 500 events with 8 independent coordinates.

*Unusual features of the program*
Complete data set of observations is not held in core since the dispersion matrix is recomputed after each record is read.

*Reference*

[1] H. Wind, Proc. Cern Summer School on Computing and Data processing, 1972.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 56–69. © NORTH-HOLLAND PUBLISHING CO., AMSTERDAM

# MULTIVARIATE LEAST SQUARES FITTING PROGRAM USING MODIFIED GRAM–SCHMIDT TRANSFORMATIONS

M.J. O'CONNELL
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Received 4 February 1974

## PROGRAM SUMMARY

*Title of program:* GSFIT

*Catalogue number:* ABCH

| *Computer:* | *Installation:* |
|---|---|
| IBM 370/195 | Rutherford Laboratory |
| ICL 1906A | Atlas Laboratory |
| CDC 6600 | CERN |

*Operating system:* IBM OS/HASP

*Programming language used:* FORTRAN

*High speed store required:* 37.5K words

*No. of bits in a word:* 32

*Overlay structure:* None

*No. of magnetic tapes required:* 1 for input

*Other peripherals used:* Card reader, lineprinter

*No. of cards in combined program and test deck:* 1411

*Keywords:* General purpose, nuclear, high energy, least squares, modified Gram–Schmidt transformations, orthogonal basis vectors, Chebyshev polynomials, Legendre polynomials, multivariate analysis.

*Nature of physical problem*
Fitting a dependent variable in terms of functions of many independent variables, e.g. finding the momentum of a charged particle from observation of its trajectory in a magnetic field.

*Method of solution*
Residual sum of squares is minimized using modified Gram–Schmidt orthogonal basis vectors.

*Restrictions on the complexity of the problem*
None in principle; coding arranged for 6 independent variables, 250 observations, up to 1000 trial functions.

*Typical running time*
15 seconds on IBM 360/195

*Unusual features of the program*
User has considerable control over the functions to be included, with the facility to reject marginally contributing terms.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 71–84. © NORTH-HOLLAND PUBLISHING CO., AMSTERDAM

# IMPROVED VERSION OF GROUP-THEORETICAL ANALYSIS OF LATTICE DYNAMICS *

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*Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87544, USA*

and

T.G. WORLTON
*Argonne National Laboratory, Argonne, Illinois 69439, USA*

Received 9 May 1974

## PROGRAM SUMMARY

*Title of program:* GROUP THEORY LATTICE DYNAMICS 2

*Catalogue number:* ACMM

| *Computer:* | *Installation:* |
|---|---|
| CDC 6600 | Los Alamos Scientific Laboratory |
| IBM 360/195 | Argonne National Laboratory |

*Operating system:* SCOPE 3.1 (LASL version)

*Programming language used:* FORTRAN IV

*High speed store required:* 137 K (octal)

*No. of bits in a word:* 60

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer

*Number of cards in combined program and test deck:* 2334

*Reference to other published version of this program:*
*Catalogue number:* ACMI; *Title:* GROUP THEORY OF LATTICE DYNAMICS: *Ref. in CPC:* 3 (1972) 82

*Keywords:* Solid state, lattice dynamics, group theory, phonons, symmetry, dispersion curves, dynamical matrix, irreducible multiplier representations, molecular vibrations, external modes, time reversal invariance, projection operators.

*Nature of physical problem*
The original version of the program [1] symmetry-reduced the dynamical matrix characterizing lattice vibrations of solids, constructed symmetry coordinates which were labeled by the irreducible multiplier representations of the group of the wavevector, and block-diagonalized the dynamical matrix. This improved version of the program allows one to calculate the symmetry properties of the external modes of vibration of molecular crystals [2], to generate the irreducible multiplier representation (IMR's) [3], and to include the effects of time reversal invariance (TRI) on the symmetry coordinates [4].

*Method of solution*
The invariance of the dynamical matrix under unitary transformations by matrices in a reducible multiplier representation of the time reversal invariant point group of the wavevector leads to a formula for the symmetry-reduction of the dynamical matrix. The projection operator method is used to construct the symmetry coordinates. The projection operator is dependent on the reducible multiplier representation used and the IMR's of the group of the wavevector. These IMR's are generated in the program by the method of orbitals from the representations of cyclic subgroups of the group of the wavevector which in turn are constructed from the roots of unity. The symmetry coordinate vectors form a matrix, which transforms the symmetry-reduced dynamical matrix into block-diagonalized form.

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* Work performed under the auspices of the U.S. Atomic Energy Commission.

*Restrictions on the complexity of the problem*
The program is dimensioned for up to 30 degrees of freedom per unit cell but this may be increased to 60. Redundant coordinates for linear molecules are not eliminated. For certain low-symmetry crystals in the trigonal and hexagonal systems, the symmetry-reduction of the dynamical matrix is incomplete because of complicated relations between elements of the matrix.

*Unusual features of the program*
By changing three cards in subroutine POASC, the symmetry coordinates can be punched out for use in calculating neutron scattering structure factors for one phonon scattering.

*Typical running time*
Calcium-tungstate, which has 18 degrees of freedom (2 atoms and 2 molecular units/cell), with 10 independent wavevectors takes 45 sec on a CDC-6600.

*References*

[1] T.G. Worlton and J.L. Warren, Computer Phys. Commun. 3 (1972) 88 and 4 (1972) 382.
[2] T.G. Worlton, Computer Phys. Commun. 4 (1972) 249.
[3] T.G. Worlton, Computer Phys. Commun. 6 (1973) 149.
[4] J.L. Warren, Phys. Rev. B9 (1974) 3603.

C-264

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 85–94. NORTH-HOLLAND PUBLISHING COMPANY

# THE HERMITIAN MATRIX EIGENPROBLEM $Hx = eSx$ USING COMPACT ARRAY STORAGE

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Received 6 March 1974

## PROGRAM SUMMARY

*Title of program:* COMPLEX GENERALIZED EIGENPROBLEM

*Catalogue number:* AAAF

| *Computer:* | *Installation:* |
|---|---|
| IBM 370/165 | Computel, Ottawa |
| IBM 360/67 | University of Alberta |
| ICL 1906A | Oxford University |
| Univac 1108 | Computel, Ottawa |

*Operating system:* OS – MVT – HASP

*Programming language used:* FORTRAN

*High speed storage required:* 125K bytes

*No. of bits in a byte:* 8

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* None

*No. of cards in combines program and test deck:* 1007

*Keywords:* General, hermitian matrix, generalized eigenproblem, Choleski decomposition, complex matrices.

*Nature of the physical problem*
The eigenproblem $Hx = eSx$, where $H$ and $S$ are complex hermitian matrices with $S$ positive definite has arisen in studies of the vibrational spectra of crystals and the molecular electronic structure of polymers.

*Method of solution*
The metric $S$ is decomposed by a complex variant of the Choleski decomposition $S = LL^{+}$, where $L^{+}$ denotes the hermitian conjugate of $L$. $L$ is a complex lower triangular matrix with real diagonal elements. The matrix $H$ is transformed to $G = L^{-1}H(L^{+})^{-1}$, so the problem is recast $Gy = ey$, where $y = L^{+}x$. $G$ is hermitian and its eigensolutions are obtained by Mueller's algorithm [1]. The complete process when carried out for real matrices $H$ and $S$ has been described by Martin and Wilkinson [2].

*Restrictions on the complexity of the problem*
Currently the program will handle matrices of order $\leqslant 40$. However, matrices of order 126 (without metric) have been solved by Birss of the University of Alberta.

*Typical running time*
CPU time required on the Computel/IBM 370/165 for the test deck consisting of one order 10 problem with metric, one order 10 problem without metric and one order 2 problem with metric was 6.77 seconds inclusive of testing. The timing is, however, altered by overall machine usage, and the same deck has been timed on a separate occasion at 5.85 seconds.

*Unusual features of the program*
The program uses a compact method for storing $H$ and $S$. A hermitian matrix $G$ may be written $G = G\mathrm{R} + \mathrm{i}G\mathrm{I}$, where $\mathrm{i} = (-1)^{1/2}$; but $G\mathrm{R}^{\mathrm{T}} = G\mathrm{R}$, and $G\mathrm{I}^{\mathrm{T}} = -G\mathrm{I}$ for $G$ hermitian, where $^{\mathrm{T}}$ denotes transposition. Note that $G\mathrm{I}_{jj} = 0$ for all $j$. If $M$ is our machine storage array, then $G_{jj} = M_{jj} + \mathrm{i}0$ for all $j$, and for $k > j$, $G_{jk} = M_{kj} + \mathrm{i}M_{jk}$, $G_{kj} = M_{kj} - \mathrm{i}M_{jk}$. This means of accessing array elements may be time consuming, particularly in a paging environment, where alternative storage mechanisms should be employed if large matrices are to be solved regularly.

*References*

[1] D.J. Mueller, Num. Math. 8 (1966) 72–92.
[2] R.S. Martin and J.H. Wilkinson, Num. Math. 11 (1968) 99–110.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 95–100. NORTH-HOLLAND PUBLISHING COMPANY

# RACAH'S OUTER MULTIPLICITY FORMULA

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and

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Received 2 May 1974

## PROGRAM SUMMARY

*Title of program:* RACOUT

*Catalogue number:* AAAG

*Computer:* IBM 370/168; *Installation:* Uni-Coll Corporation

*Operating system:* HASP-II

*Programming language used:* FORTRAN IV

*High speed store required:* 62,540 words

*No. of bits in a word:* 16

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals:* Card reader, line printer

*No. of cards in combined program and test deck:* 670

*CPC Library subprograms used:*

| *Catalogue number:* | *Title:* | *Ref. in CPC:* |
|---|---|---|
| AAAA | FREUD | 6 (1973) 24 |

*Keywords:* General, Lie algebra, outer multiplicity, irreducible representation, Racah's formula.

*Nature of the physical problem*
To find the decomposition of the tensor product of two irreducible representations of a complex simple Lie algebra into a direct sum of irreducible representations.

*Method of solution*
The weight diagram of the smaller dimensioned representation is generated using Dynkin's algorithm and Freudenthal's formula. The highest weight of any irreducible component of the tensor product of the given representations with highest weights $\lambda'$ and $\lambda''$ can be written as $\mu + \lambda''$ where $\mu$ is a member of the weight system of $\lambda'$ (assumed to be the smaller dimensioned representation). All sums $\mu + \lambda''$ are formed and if $\mu + \lambda''$ is dominant, Racah's formula is used to compute its outer multiplicity.

*Restrictions on the complexity of the problem*
The program handles all Lie algebras of rank $\leqslant 9$. The smaller dimensioned representation must have no more than 1000 weights.

*Typical running times*
The first (ordered by dimension) ten nontrivial pairs of representations for the Lie algebra $B_3$ ran in 1.2 seconds.

*Unusual features of the program*
An efficient method [1] of truncating the sum over the Weyl group is used so that only a small number of terms need be taken even when the Weyl group has order greater than $10^6$. By using the IBM 360 Fortran IV IMPLICIT statement all variables in the program are declared to be integers. When running on computers other than IBM 360 and 370 series, variables not beginning with I to N will have to be declared as type INTEGER.

*Reference*

[1] Bernard Kolman and Robert E. Beck, J. Comput. Phys. 13 (1973) 161–163.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 101–117. NORTH-HOLLAND PUBLISHING COMPANY

# WEIZMANN SHELL MODEL COMPUTATIONAL CODE

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Received 10 April 1974

## PROGRAM SUMMARY

*Title of program*: WSMCC

*Catalogue number*: ABGN

*Computer*: IBM 370/165; *Installation*: Weizmann Institute of Science, Israel

*Operating system*: OS360

*Programming language used*: FORTRAN IV

*High speed storage required*: 7000 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: One

*Other peripherals used*: Card-reader and printer

*No. of cards in combined program and test deck*: 5695

*CPC Library subprograms used*:
*Catalogue number*: ABKB; *Title*: JJTCFP; *Ref. in CPC*: 1 (1970) 225.

*Keywords*: Nuclear, cfp, wave functions, shell-model, *j–j* coupling, seniority, spin, isospin, configuration, coupling, recoupling of angular momenta.

*Nature of physical problem*
WSMCC is a computer program which carries out nuclear shell-model (spectroscopy) calculations. Given the total number of particles, total angular momentum and total isospin, the program calculates the energy levels and eigenstates as functions of the two-body matrix elements and the single particle energies.

*Method of solution*
Calculations are carried out by reducing the problem to the two-body matrix elements, using the well-known shell-model formalism presented in ref. [1]. The current version of the program can handle large configurations as well as small ones, and it is able to calculate any matrix element of a two-body scalar operator in one, two or three shells. For more than three shells, the program can be extended by recoupling the angular momenta of the $n$ particles in the wave function so that all unchanged $(n-2)$ particles will be coupled together (this extension is available, but is not included in the current version).

*Restrictions on the complexity of the problem*
Calculations are done in double-precision mode (each number occupies two 32-bit words in memory). The above mentioned high speed storage size includes an array of about 6500 cfp's and a hamiltonian matrix of 45 by 45. In case of a larger matrix, the elements are written out as they are computed for later diagonalization.

*Typical running time*
Running time depends roughly on the square of the order of the hamiltonian matrix, the values of total and intermediate spins and isospins; number of particles and configurations; the spin of the configuration; whether the calculation is completed in core or not; whether the classification of the states is read in or calculated by the program; and many others. To give an order of magnitude for the running time we mention that for the calculation of the 21 states of $^{36}$Ar with zero angular momentum and isospin, the present version needs about 13 sec on an IBM 370/165; the same calculation for the 325 states (with $J = 0$ and $T = 0$) of $^{24}$Mg needs about 20 min and for the 21 states of $^{20}$Ne only 2 sec. So it is quite meaningless to speak about a "typical" running time.

*Unusual features of the program*
The input coefficients of fractional parentage (cfp) cards can be taken with their original format from ref. [2]. Most of the subroutines can be used alone for different calculations using the shell-model formalism.

*References*

[1] A. de Shalit and I. Talmi, *Nuclear shell theory* (Academic Press, New York, 1963).
[2] L.B. Hubbard, Computer Phys. Commun. 1 (1970) 225.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 118–122. NORTH-HOLLAND PUBLISHING COMPANY

# TIMER - A SOFTWARE INSTRUMENTATION ROUTINE FOR MAKING TIMING MEASUREMENTS

M.H. HUGHES and A.P.V. ROBERTS
*UKAEA Culham Laboratory, Abingdon, Berkshire, UK*

Received 2 January 1974

## PROGRAM SUMMARY

*Title of program*: TIMER

*Catalogue number*: ABUH

*Computer*: ICL System 4/70; *Installation*: UKAEA Culham Laboratory

*Operating system*: Multijob

*Programming language used*: Fortran

*High speed storage required*: 28440 kbytes*

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Lineprinter

*No. of cards in combined program and test deck*: 545

* for test program.

*Keywords*: General purpose, instrumentation, timing.

*Nature of physical problem*
TIMER is an instrumentation routine which measures and records the CPU time spent in various sections of a program, so that effort spent in optimization can be concentrated where it will be most effective.

*Method of solution*
Appropriate calls to the Fortran IV routine TIMER are used to switch set of up to 50 software clocks on and off and print details as required. A correction is made for time spent in the routine itself and in the supervisor.

*Restrictions on the complexity of the problem*
TIMER can be used on any computer system for which a suitable hardware clock is available, provided that the call to this clock is modified appropriately and the necessary timing corrections measured and inserted.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 123–129. NORTH-HOLLAND PUBLISHING COMPANY

# OLYMPUS RESTART FACILITIES

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Received 12 March 1974

## PROGRAM SUMMARY

*Title of program*: LEDGER

*Catalogue number*: ABUI

*Computer*: ICL System 4/70; *Installation*: Culham Laboratory

*Operating system*: Multijob

*Programming language used*: FORTRAN

*High speed storage required*: 44 K bytes*

*No. of bits in a byte*: 8

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Line printer

*No. of cards in combined program and test deck*: 571

*Keywords*: General purpose, restart, ledger.

*Nature of physical problem*

Large scientific computer programs are often required to write periodic records to some output device so that a run may be stopped and restarted. The package described here provides general-purpose facilities for doing this, which are largely independent both of the program and also of the computer on which it is run.

*Method of solution*

Selected COMMON blocks of a Fortran program are written to or read from a 'ledger file'. A library subroutine called LEDGER is provided, written in Standard Fortran [1], which performs various operations on this file. All the individual user has to do is to supply his own version of a simple ad hoc subroutine called RECORD which defines the blocks to be transmitted.

*Restrictions on the complexity of the problem*

The package is intended primarily for use under the OLYMPUS [2–4] system for initial-value Fortran programs, and communication is via labelled COMMON. Because Standard Fortran makes no provision [1] for detecting end-of-file or error conditions, a non-standard READ statement has been used which is available on ICL and IBM computers. This however does not appear in LEDGER itself but only in two small subroutines RECO and RECNUM which are easily changed, and we explain how to make the necessary changes for CDC computers as an example. The package also includes an assembler language subroutine UPDATE which obtains housekeeping information from the supervisor and must be recoded for a different type of computer system.

*References*

[1] *Standard Fortran Programming Manual*, Computer Standard Series, National Computing Centre Ltd., Manchester, England (1970).

[2] J.P. Christiansen and K.V. Roberts, Computer Phys. Commu 7 (1974) 245.

[3] M.H. Hughes and K.V. Roberts, OLYMPUS and Preprocessor Package for an IBM 370/165, Computer Phys. Commun (1974, to be submitted).

[4] M.H. Hughes and K.V. Roberts, OLYMPUS for the CDC 6500, Computer Phys. Commun. (1974, to be submitted).

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* for test program.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 130–140. NORTH-HOLLAND PUBLISHING COMPANY

# PIRK: A COMPUTER PROGRAM TO CALCULATE THE ELASTIC SCATTERING OF PIONS FROM NUCLEI‡

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*Pittsburgh, Pennsylvania 15213, USA*

Received 13 June 1974

## PROGRAM SUMMARY

*Title of program*: PIRK

*Catalogue number*: ABCJ

*Computer*: UNIVAC 1108; *Installation*: Computer Center, Carnegie–Mellon Univ., Pittsburgh, Pa. 15213. Program has also run on IBM 360/67, CDC 6600, DEC PDP-11/45 and PDP-10

*Operating system*: Univac EXEC II

*Programming language used*: FORTRAN IV

*High speed storage required*: 22,692 words

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader and line printer

*No. of cards in combined program and test deck*: 778

*Keywords*: Nuclear, pion, elastic scattering, angular distribution, optical model, Klein–Gordon, Runge–Kutta, complex potential, phase shift, cross section.

*Method of solution*

Angular distributions for the elastic scattering of pions from optical potential representations of the nucleus are generated from the partial wave expansion of the scattering amplitude. Complex phase shifts for each partial wave are obtained by numerically integrating the radial Klein–Gordon equation in the interior region and matching to the asymptotic Coulomb wavefunction in the exterior region. The integration is done using the fourth-order Runge–Kutta method. To insure accuracy, the program utilizes double precision arithmetic. Several optical potentials and nuclear densities are available in the program.

*Restrictions on the complexity of the program*

A maximum of 50 partial waves may be included in the scattering amplitude without changing the program. The program presently treats only a restricted class of non-local potentials; other types of non-localities may be of physical interest. The finite size, spherical nuclear charge density is that of a uniform sphere.

*Typical running time*

Depends on the number of integration steps per partial wave and the number of partial waves. The test case given requires 2.9 seconds on the UNIVAC 1108. (15 partial waves, 200 integration steps per partial wave.)

## ERRATUM NOTICE

*Title of manuscript*: Irreducible multiplier representations

*Author*: T.G. Worlton

*Reference*: Computer Phys. Commun. 6 (1973) 149

*Title of program*: IMR CALCULATION

*Catalogue number*: ACMI0002

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 149–198. NORTH-HOLLAND PUBLISHING COMPANY

# A GENERAL PROGRAM TO CALCULATE ATOMIC CONTINUUM PROCESSES USING THE *R*-MATRIX METHOD

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Received 9 July 1974

## PROGRAM SUMMARY

*Title of program*: RMATRX STG1

*Catalogue number*: AAHA

| *Computer*: | *Installation*: |
|---|---|
| ICL 1906A | Atlas Computer Laboratory, Chilton, Didcot, Berkshire, England |
| IBM 370/195 | Rutherford Laboratory, Chilton, Didcot, Berkshire, England |

*Operating system*: GEORGE 4

*Programming language used*: FORTRAN IV

*High speed storage required*: 118, 592 words

*No. of bits in a word*: 24 for integer variable, 2 words per floating point variable

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, scratch disc store, permanent disc store

*No. of cards in combined program and test deck*: 3799

*CPC Library subprograms used*:

| *Catal. number* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAHE | A NEW VERSION OF BASFUN | This paper |
| AAHB | RMATRX STG2 | This paper |
| AAHC | RMATRX STG3 | This paper |

*Keywords*: Atomic, electron–atom scattering, electron–ion scattering, photoionization, polarizability, *R*-matrix, continuum, bound, pseudo-potential, de Vogelaere's method, radial integrals, *RK* integrals.

*Nature of the physical problem*
This program calculates all one-electron, two-electron and multipole radial integrals involving the bound and continuum orbitals necessary to enable electron–atom or –ion scattering, photoionization or frequency dependent polarizabilities to be calculated for a general atomic system [1, 2]. The bound orbitals are specified analytically. The continuum orbitals are calculated by the program. The integrals are stored on a permanent tape or disc file for use by RMATRX STG2 [3].

*Method of solution*
The continuum orbitals are determined by integrating numerically a differential equation with a given potential using de Vogelaere's method and subject to *R*-matrix boundary conditions. The one-electron integrals and the multipole integrals are evaluated numerically using Simpson's rule. The *RK* integrals are determined by solving a differential equation and then using Simpson's rule.

*Restrictions on the complexity of the program*
Up to 5 bound orbitals and 20 continuum orbitals for each angular momentum can be included. More orbitals can be included by recompiling with larger dimensions. Certain arrays which contain the radial integrals may have to have their dimensions increased for large runs.

*Typical running time*
The running time depends approximately on the square of the number of bound orbitals, on the square of the number of continuum orbitals for each angular momentum and on the number of continuum angular momenta. The test run took 500 seconds on the ICL 1906A which is equivalent to about 50 seconds on the IBM 370/195.

*References*

[1] P.G. Burke, A. Hibbert and W.D. Robb, J. Phys. B4 (1971) 153.
[2] D.C.S. Allison, P.G. Burke and W.D. Robb, J. Phys. B5 (1972) 55.
[3] K.A. Berrington, P.G. Burke, J.J. Chang, A.T. Chivers, W.D. Robb and K.T. Taylor, Computer Phys. Commun. 8 (1974) 149 (this paper).

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* Now at Joint Institute for Laboratory Astrophysics, Boulder, Colorado, USA.

## PROGRAM SUMMARY

*Title of program*: RMATRX STG2

*Catalogue number*: AAHB

| *Computer*: | *Installation*: |
|---|---|
| ICL 1906A | Atlas Computer Laboratory, Chilton, Didcot, Berkshire, England |
| IBM 370/195 | Rutherford Laboratory, Chilton, Didcot, Berkshire, England |

*Operating system*: GEORGE 4

*Programming language used*: FORTRAN IV

*High speed storage required*: 96,256 words

*No. of bits in a word*: 24 for integer variable, 2 words per floating point variable

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, scratch disc store, permanent disc store

*No. of cards in combined program and test deck*: 3780

*CPC Library subprograms used*:

| *Catal. number* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACRN | A NEW D SHELL C.F.P. | 6 (1973) 88 |
| ACQB | P SHELL C.F.P. | 1 (1969) 15 |
| ACQV | WEIGHTS NEW VERSION | 2 (1971) 180 |
| ACQV0001 | ADAPT WEIGHTS FOR ONE-ELECT | 7 (1974) 318 |
| AAHD | A NEW VERSION OF NJSYM | This paper |
| AAKF | REDUCED TENSOR MATRIX ELEMENTS | 6 (1973) 132 |
| AAHA | RMATRX STG1 | This paper |
| AAHC | RMATRX STG3 | This paper |

*Keywords*: Atomic, electron–atom scattering, electron–ion scattering, photoionization, polarizability, $R$-matrix, hamiltonian matrix, ionic, Racah coefficient, fractional parentage coefficient, recoupling, angular integral, continuum, bound, $LS$ coupling, long-range potentials, dipole matrix elements.

*Nature of the physical problem*
This program reads the radial integrals stored on a permanent tape or disc file by RMATRX STG1 [1]. It then calculates the hamiltonian matrix elements, the asymptotic potential coefficients and the dipole length and velocity matrix elements from a given initial state to the final state specified by $LS$ and the channel quantum numbers. These quantities are stored on a permanent tape or disc file for use by RMATRX STG3 [1].

*Method of solution*
The triangular relations are used to determine the number of coupled channels given the value of $L$ and $S$ and the quantum numbers of the atomic states. The angular integrals are carried out using the methods of Racah algebra. These are then combined with the radial integrals evaluated by RMATRX STG1.

*Restrictions on the complexity of the program*
Up to 20 continuum orbitals for each angular momentum can be included. This number can be increased by recompiling. The program assumes that $L$ and $S$ are good quantum numbers and neglects effects due to the spin–orbit interaction.

*Typical running time*
The running time depends on the square of the number of shells and the number of configurations included but in general a single run of STG2 is usually an order of magnitude or more shorter than the STG1 run. The test run took 25 seconds on the ICL 1906A.

*References*

[1] K.A. Berrington, P.G. Burke, J.J. Chang, A.T. Chivers, W.D. Robb and K.T. Taylor, Computer Phys. Commun. 8 (1974) 149 (this paper).

## PROGRAM SUMMARY

*Title of program*: RMATRX STG3

*Catalogue number*: AAHC

| *Computer*: | *Installation*: |
|---|---|
| ICL 1906A | Atlas Computer Laboratory, Chilton, Didcot, Berkshire, England |
| IBM 370/195 | Rutherford Laboratory, Chilton, Didcot, Berkshire, England |

*Operating system*: GEORGE 4

*Programming language used*: FORTRAN IV

*High speed storage required*: 78,336 words

*No. of bits in a word*: 24 for integer variable, 2 words per floating point variable

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, scratch disc store, permanent disc store

*No. of cards in combined program and test deck*: 3554

*CPC Library subprograms used*:

| *Catal. number* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAHE | A NEW VERSION OF BASFUN | This paper |
| ACRK | ASYM VERSION FOR ICL 1900 | 5 (1973) 416 |
| AAHA | RMATRX STG1 | This paper |
| AAHB | RMATRX STG2 | This paper |

*Keywords*: Atomic, electron–atom scattering, electron–ion scattering, polarizability, *R*-matrix, hamiltonian matrix, Householder method, eigenvalues, eigenvectors, cross-sections, Buttle correction, De Vogelaere's method, phase shifts, *K*-matrix, long-range potentials, asymptotic solutions, WBK.

*Nature of the physical problem*

This program reads the hamiltonian matrix elements etc. stored on a permanent tape or disc file by RMATRX STG2 [1]. It then diagonalizes this matrix and calculates the *R*-matrix and the Buttle correction. Then either the electron atom or ion cross-section, the photoionization cross-section or the frequency dependent polarizability for a range of incident energies or frequencies is calculated.

*Method of solution*

The Householder method and the bisection method are used to diagonalize the hamiltonian matrix and the Buttle correction is calculated by solving a differential equation using de Vogelaere's method. In the case of electron scattering and photoionization the coupled differential equations are solved in the asymptotic region using either an asymptotic series expansion or a WBK solution. The *K*-matrix and *T*-matrix are determined from the *R*-matrix by matrix algebra.

*Restrictions on the complexity of the program*

The maximum size of the hamiltonian matrix that can be treated is 120, the maximum number of channels is 6 and the maximum number of energies which can be dealt with in one run is 50. All of these can be increased by recompiling.

*Typical running time*

For hamiltonian matrices of order or greater than about 100 the time is dominated by the diagonalization procedure. For smaller matrices the time taken to solve the electron scattering equations in the asymptotic region is usually the dominating factor if more than a few energy points are required. The test runs took 55 seconds for electron scattering, 54 seconds for photoionization and 10 seconds for polarizability on the ICL 1906A.

*References*

[1] K.A. Berrington, P.G. Burke, J.J. Chang, A.T. Chivers, W.D. Robb and K.T. Taylor, Computer Phys. Commun. 8 (1974) 149 (this paper).

## PROGRAM SUMMARY

*Title of program*: A NEW VERSION OF NJSYM

*Catalogue number*: AAHD

| *Computer*: | *Installation*: |
|---|---|
| ICL 1906A | Atlas Computer Laboratory, Chilton, Didcot, Berkshire, England |
| IBM 370/195 | Rutherford Laboratory, Chilton, Didcot, Berkshire, England |

*Operating system*: GEORGE 4

*Programming language used*: FORTRAN IV

*High speed storage required*: 11,264 words

*No. of bits in a word*: 24 for integer variable, 2 words per floating point variable

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1580

*Reference to other published version of this program*:
*Catalogue number*: AAGD; *Title*: NJSYM; *Ref. in CPC*: 1 (1969) 241

*Keywords*: Atomic, nuclear, structure, scattering, recoupling coefficient, Racah coefficient, Wigner coefficient, Fano coefficient, rotation group, 3-*j* symbol, 6-*j* symbol, 9-*j* symbol, 12-*j* symbol, 15-*j* symbol, 18-*j* symbol, 21-*j* symbol, angular momentum, matrix element, angular integral, representation of three-dimensional rotation.

*Nature of physical problem*

This is a new version of the program by Burke [1]. It combines the latter with a correction by Burke [2] and adaptations by Hibbert [3] and Grant [4]. The following minor modifications, which do not affect the operation of the program materially, have also been made:

(i) The real constants have been replaced by real variables which are initialized in DATA statements. This facilitates the conversion from single precision to double precision.

(ii) The integer variables used for dimension checks are now initialized in the directing program instead of in SUBROUTINE NJSYM. KFL7 has been added to COMMON block IMEN to check the dimension of the J1 array. The latter was previously incorrectly checked using KFL4. In addition KFL2 and KFL5 have been increased to 100 and 200 respectively and the appropriate arrays increased. This allows more extensive runs to be carried out.

*References*

[1] P.G. Burke, Computer Phys. Commun. 1 (1969) 241.
[2] P.G. Burke, Computer Phys. Commun. 2 (1971) 173.
[3] A. Hibbert, Computer Phys. Commun. 2 (1971) 181.
[4] I.P. Grant, Computer Phys. Commun. 5 (1973) 161.

## PROGRAM SUMMARY

*Title of program*: A NEW VERSION OF BASFUN

*Catalogue number*: *AAHE*

| *Computer*: | *Installation*: |
|---|---|
| ICL 1906A | Atlas Computer Laboratory, Chilton,Didcot, Berkshire, England |
| IBM 370/195 | Rutherford Laboratory, Chilton, Didcot, Berkshire, England |

*Operating system*: GEORGE 4

*Programming language used*: FORTRAN IV

*High speed storage required*: 24,576 words

*No. of bits in a word*: 24 for integer variable, 2 words per floating point variable

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 956

*Reference to other published version of this program*:
*Catalogue number*: ACQS; *Title*: NUMERICAL ORBITAL FUNCTIONS; *Ref. in CPC*: 1 (1970) 457

*Keywords*: Atomic, nuclear, basis functions, continuum, bound, Bessel functions, Yukawa, static, square well, De Vogelaere, *R*-matrix, eigenfunction.

*Nature of the physical problem*
This is a new version of the program by Robb [1]. The program has been changed to conform with ASA Fortran and to become a compatible unit with the atomic scattering packages [2] being run on the Atlas Computer Laboratory ICL 1906A and the Rutherford Laboratory IBM 370/195. The changes are as follows:

(i) Replacement of several non-standard FORTRAN statements.
(ii) Reordering of the variables in the COMMON blocks containing both real and integer variables so that the program can be run in single or double precision on the IBM 370/195. The real variables precede the integer variables.
(iii) Replacement of all real constants that occur in the program with real variables. The latter are initialized in data statements. This facilitates the conversion from single precision to double precision.
(iv) The subrountine MA01A has been replaced by a fully commented and improved version.
(v) Some additional tests for zero are inserted to prevent overflow.

*References*

[1] W.D. Robb, Computer Phys. Commun. 1 (1970) 457.
[2] K.A. Berrington, P.G. Burke, J.J. Chang, A.T. Chivers, W.D. Robb and K.T. Taylor, Computer Phys. Commun., 8 (1974) 149 (this paper).

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COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 199–219. NORTH-HOLLAND PUBLISHING COMPANY

# "MIA", A FORTRAN-IV PROGRAM FOR MAKING SPIN AND PARITY ASSIGNMENTS TO HIGH-LYING SINGLE AND COHERENT TWIN NUCLEAR LEVELS FROM (ALPHA, NUCLEON) ANGULAR DISTRIBUTIONS IN ON-RESONANCE, COMPOUND-NUCLEAR, CHANNEL-SPIN-$\frac{1}{2}$ REACTIONS ‡

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and

H.R. HIDDLESTON
*Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA*

Received 29 July 1974

## PROGRAM SUMMARY

*Title of program*: MIA

*Catalogue number*: ABMI

*Computer*: Digital PDP-9 or CDC-6600; *Installation*: PDP-9 at Nuclear Center, Lowell Technological Institute, Lowell, Mass., USA; CDC-6600 at Computation Center, University of Texas at Austin, Austin, Texas, USA

*Operating system*: PDP-9 advanced software system

*Programming languages used*: FORTRAN-IV

*High speed store required*: 24 Kwords.

*No. of bits in word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Disc or dectape (optional), card reader, line printer, storage display oscilloscope, microfilm unit (optional), teletype console

*No. of cards in combined program and test deck*: 1360

*Keywords*: Nuclear, spectroscopy, spin–parity assignments, reactions, channel spin, resonance, compound nucleus, single-level, twin-level resonances, angular distribution, differential cross section, distribution function, Legendre polynomial, vector momentum coupling, display oscilloscope, storage oscilloscope, plotted print-out.

*Nature of physical problem*
Nuclear spectroscopy yielding spin and parity assignments to high-lying compound nuclear levels is facilitated by the study of angular distributions from on-resonance reactions involving channel-spin-$\frac{1}{2}$ (or spin-0) incoming and outgoing interaction channels. For pure single-level or coherent twin-level resonances the spin–parity assignments can be deduced from a direct graphic comparison of measured and calculated angular distributions for, e.g., (alpha, nucleon) reactions on spin-$\frac{1}{2}$ target nuclei leading to spin-0 residual nuclear states. The program "MIA" is designed to accomplish this task, taking into account entrance and exit barrier penetrabilities, the effect of competing outgoing reaction channels and, if desired, spin-orbit coupling; it features oscilloscope display, external parameter manipulation and plotted print-out facilities that permit interactive communication between the operator and the data.

*Method of solution*
At option the program can range from consideration of a single, pure, resonance angular distribution to a cyclic sequence of 1015 possible combinations of parameters specifying single-level and coherent twin-level involvement, displaying the experimental and theoretical results graphically on an oscilloscope screen for direct comparison of shape and magnitude, with opportunity for parameter variation from the console teletype

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‡ Work supported in part by the U.S. Atomic Energy Commission and National Science Foundation.

keyboard. Selected results can at will be printed out in tabular and plotted form for subsequent reference.

### *Restrictions on the complexity of the problem*

The program is designed to cater for half-integer-spin states in the compound nucleus ranging from $\frac{1}{2}$ to $\frac{13}{2}$ of either parity; it has specifically been compiled for consideration of channel-spin-$\frac{1}{2}$ on-resonance reactions induced by alpha particles, of the type $\frac{1}{2}^{\pm}(\alpha,\mathcal{N})0^{+}$. Hence the orbital momenta are restricted to $l_{\max} \leqslant 6$.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 220–235. NORTH-HOLLAND PUBLISHING COMPANY

# A FIXED CORE HARTREE–FOCK PROGRAM FOR CALCULATING BOUND AND CONTINUUM ORBITALS

G.N. BATES

*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Northern Ireland*

Received 12 August 1974

## PROGRAM SUMMARY

*Titel of program*: FIXED CORE HARTREE–FOCK

*Catalogue number*: ACRX

| *Computer*: | *Installation*: |
|---|---|
| IBM 360/65 | University of Windsor, Windsor, Ontario, Canada |
| ICL 1906 A | Atlas Computer Laboratory, Chilton, Didcot, Berkshire, England |

*Programming language used*: FORTRAN IV

*High speed storage required*: 46K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, printer, disc (scratch files), punch (optional)

*No. of cards in combined program and test deck*: 2140

*Keywords*: Atomic orbital, bound state, continuum state, numerical Hartree–Fock, wave function.

*Nature of physical problem*
Numerical 'fixed core' or 'frozen core' Hartree–Fock results are determined for one bound or continuum orbital of an atom.

*Method of solution*
The Hartree–Fock equation is converted to an integral equation and numerically integrated. Exchange terms are included through Marriott's method [1].

*Restrictions on the complexity of the problem*
The energy of the continuum electron is restricted (by numerical error) to a few hundred eV. If large atoms are attempted, shortage of computer time may also impose a restriction.

*Typical running time*
The CPU time for the test case was 90 seconds on Large Core Storage (slow core) or approximately 15 seconds on Main Core (fast core).

*Reference*
[1] R. Marriott, Proc. Phys. Soc. 72 (1958) 121.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 236–245. NORTH-HOLLAND PUBLISHING COMPANY

# ANALYSIS OF THE INTENSITY DISTRIBUTION IN THE ROTATIONAL STRUCTURE OF THE ELECTRONIC SPECTRA OF DIATOMIC MOLECULES BY COMPUTER SIMULATION

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*FOM-Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands*

Received 26 April 1974

## PROGRAM SUMMARY

*Title of program*: ROSCOS

*Catalogue number*: ACRW

*Computer*: El-X8; *Installation*: Mathematisch Centrum, Amsterdam, The Netherlands

*Operating system*: MILLI

*Programming language used*: ALGOL 60

*High speed storage required*: 39458 words

*Number of bits in a word*: 27

*Overlay structure*: None

*Number of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, plotter

*Number of cards in combined program and test deck*: 1266

*Keywords*: Molecular, diatomic, wavelength, line-strengths, intensity, convolution, plotting of spectrum, rotational band spectrum.

*Nature of the physical problem*

This program is concerned with the analysis of the intensity distribution in the rotational structure of the CH($A^2\Delta - X^2\Pi$) spectrum, produced by dissociative excitation of simple aliphatic hydrocarbons ($CH_4$, $C_2H_2$, $C_2H_4$, $C_2H_6$) by electron impact.

*Method of solution*

If the resolving power of the monochromator does not allow one to separate all lines contributing to the spectrum, the intensity distribution in the rotational structure can be established by simulation of the experimental spectrum on the computer by a convolution technique. For this purpose, the wavelengths, line-strengths and intensities of the rotational transitions are calculated. Relevant formulae are given by Kovács [1]. The wavelengths, which have been determined experimentally by Gerő [2], are read in. The intensity is calculated by applying a Boltzmann distribution over the rotational levels.

*Restrictions on the complexity of the problem*

The program is restricted to the calculation of a $A^2\Delta - {}^2\Pi$ transition. It can also be applied to singlet–singlet and other doublet–doublet transitions, when relevant parts of the formulas are changed (see ref. [1]).

*Typical running time*

The running time depends on the number of lines to be convoluted. The test run required 225 sec for 1714 lines, including compilation, loading and syntax control.

*References*

[1] I. Kovács, *Rotational structure in the spectra of diatomic molecules* (Adam Hilger Ltd., London, 1969).

[2] L. Gerő, Z. Phys. 118 (1941) 27.

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* Present address: Philips' Research Laboratories, Eindhoven, The Netherlands.

‡ Department of Theoretical Organic Chemistry, University of Leyden, The Netherlands.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 246–256. NORTH-HOLLAND PUBLISHING COMPANY

# FRACTIONAL PARENTAGE COEFFICIENTS FOR EQUIVALENT f SHELL ELECTRONS

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*School of Physics and Applied Mathematics,*
*The Queen's University of Belfast, Belfast BT7 1NN, N. Ireland*

Received 11 July 1974

## PROGRAM SUMMARY

*Title of program*: F SHELL C.F.P.

*Catalogue number*: ACRY

*Computer*: ICL 1906S; *Installation*: Queen's University, Belfast, N. Ireland

*Operating system*: GEORGE 3

*Programming language used*: FORTRAN IV

*High speed storage required*: 18,560 words

*No. of bits in a word*: 24

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1825

*Keywords*: Atomic, nuclear, LS coupling, fractional parentage coefficient, seniority, group representation symbols.

*Nature of the physical problem*
The CFPF package evaluates the Racah coefficients [1] of fractional parentage for equivalent f-shell electrons. These coefficients are defined by $(f^n \alpha SL|\}f^{n-1}\alpha' S'L', f\,SL)$ where $n$ denotes the number of equivalent electrons and $S, L; S'L'$ are respectively the total spin and total orbital angular momentum quantum numbers of the state in question and its parent state. The parameters $\alpha$ and $\alpha'$ are labels which are used to identify the remaining quantum numbers which are necessary for the unambiguous classification of the multiplets $f^n$ and $f^{n-1}$.

*Method of solution*
Racah [2] has shown that fractional parentage coefficients may be factored if the states to which they refer correspond to his group theoretical classification scheme. In the case of the f shell, the fractional parentage coefficients are the product of three factors. In this program all the possible factors arising in the calculation have been encoded in tabular form and placed in a block data segment. When all the quantum numbers of the state in question and its parent state have been identified, the corresponding fractional parentage coefficient is found by searching through each of three tables to pick out the required factors.

*Typical running time*
Much smaller than 1 second for one fractional parentage coefficient.

*References*

[1] G. Racah, Phys. Rev. 63 (1943) 367.
[2] G. Racah, Phys. Rev. 76 (1949) 1352.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 307–319. © NORTH-HOLLAND PUBLISHING CO., AMSTERDAM

# A NUMERICAL CODE FOR MULTIPLE "WATER BAG" GRAVITIONAL SYSTEMS

S. CUPERMAN and A. HARTEN

*Department of Physics and Astronomy, Tel-Aviv University, Tel-Aviv, Ramat-Aviv, Israel*

Received 27 March 1974

## PROGRAM SUMMARY

*Title of program:* WATER BAG MODEL

*Catalogue number:* ACRU

*Computer:* CDC 6600; *Installation:* Tel-Aviv University, Israel

*Operating system:* Scope 3.3

*Programming languages used:* Fortran

*High speed store required:* CM 150,000 words

*No. of bits in word:* 60

*Overlay structure:* None

*No. of magnetic tapes required:* Two

*Other peripherals used:* Line printer

*No. of cards in combined program and test deck:* 900

*Keywords:* Astrophysics, plasma physics, self-gravitating systems, water bag distributions, nonhomogeneous Vlasov systems, one-dimensional, distribution function.

*Nature of physical problem*

The *non-linear* stability analysis and evolution of *non-homogeneous* collisionless many-body systems are, as yet, unsolved problems. In fact, even a rigorous linear analysis is missing. This is true for both self-gravitating systems of stars and plasmas (thermonuclear or astrophysical) [1, 2]. The reason for this is that the mathematical methods available so far are not able to treat such complex problems as the non-homogeneous systems mentioned above.

*Method of solution*

A convenient numerical integration method for studying the collective bahavior of a strongly non-homogeneous, finite size, non-maxwellian system is to follow the motion of the boundary curves defining the system in phase space. This method of integration enables us to investigate a *system possibly consisting of a very large number of particles (enclosed by a boundary curve) without having to treat them explicitly.* The method was first proposed by Roberts and Berk [2] who also applied it to the study of the two-stream instability in one-dimensional plasma systems. This paper describes the computer code developed to investigate one-dimensional, collisionless systems of stars, consisting of regions of constant density matter (*in phase space*).

*Restrictions on the complexity of the problem*

The code may be used only for the investigation of one-dimensional (two-dimensional phase space), collisionless systems of stars consisting of regions of constant density matter (in phase space).

*Typical running time*

Execution times depend on the number of Eulerian strips used and on the number of mark points required to describe the system with the desired accuracy. If the number of Eulerian strips used is 215, the execution time per timestep for one mark point is about $1.5 \times 10^{-3}$ sec.

*References*

[1] S. Cuperman, A. Harten and M. Lecar, Astrophysics and Space Science 13 (1971) 425.

[2] K.V. Roberts and H.L. Berk, Phys. Fluids 10 (1967) 1595.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 320–328. NORTH-HOLLAND PUBLISHING COMPANY

# COMPUTER GENERATION OF CONNECTED GRAPHS

D.C. RAPAPORT

*Physics Department, Bar–Ilan University, Ramat-Gan, Israel*

Received 26 June 1974

## PROGRAM SUMMARY

*Title of program*: GRAFFITI

*Catalogue number*: ACOA

*Computer*: IBM 360/50; *Installation*: Bar–Ilan University

*Operating system*: HASP/OS/MFT

*Programming language used*: FORTRAN IV

*High speed storage required*: 20K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, scratch disk, card punch (optional)

*No. of cards in combined program and test deck*: 635

*Keywords*: Solid state, statistical mechanics, cluster expansions, cooperative pjenomena, critical exponents, diagrammatic expansions, ferromagnetism, graphical enumeration, Ising model, lattice statistics, perturbation theory, phase transitions, series expansions.

*Nature of the physical problem*

The most successful technique currently used in studying the behaviour of magnetic spin models (e.g., the Ising model) near their phase transitions is the series expansion method [1]. Generation of the coefficients of these expansions requires the availability of a list of suitable graphs, the type of graph required depending on the quantity being expanded. The computer program described here generates the connected graphs used in a study of the Ising model with impurities [2]. Graphs required for other kinds of perturbation expansion in statistical mechanics, quantum electrodynamics, or many-body theory, can either be obtained from this list of connected graphs, or generated directly using appropriately modified versions of the program.

*Method of solution*

Graphs are generated iteratively in order of increasing edge and vertex numbers by adding additional edges to already existing graphs. The problem is to do this efficiently and, because most graphs can be generated in more than one way, to ensure that the graphs in the final list are all distinct. The degree of overgeneration is reduced by taking into account the graph symmetry, and the problem of determining whether or not graphs are distinct is overcome by developing a canonical labelling scheme for the graphs.

*Restrictions on complexity*

The maximum graph size is set by the array dimensions and the scheme used in packing the graph adjacency matrices. Both are easily altered. The real limitation is execution time due to the rapid increase in graph numbers as more edges are added.

*Typical running times*

709 graphs with 7 vertices and 6 to 13 edges were generated in approx. 500 sec, and 834 graphs with 8 vertices and 7 to 10 edges in approx. 1000 sec on the IBM 360/50 computer.

*References*

[1] C. Domb and M.S. Green (eds.), *Phase transitions and critical phenomena*, vol. 3 (Academic Press, London, 1974).

[2] D.C. Rapaport, J. Phys. C 5 (1972) 1830, 2813.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 329–332. NORTH-HOLLAND PUBLISING COMPANY

# ADAPTATION OF A GENERAL PROGRAM TO CALCULATE ANGULAR MOMENTUM INTEGRALS IN ATOMIC STRUCTURE: INCLUSION OF THE CHECKING OF THE CONFIGURATION DATA

A. HIBBERT

*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, Northern Ireland*

Received 18 June 1974

## ADAPTATION SUMMARY

*Title of adaptation*: ADAPT TO TEST CONFIG DATA

*Adaptation number*: 0002

*Reference to original program*: Catalogue number ACQV: *title*: WEIGHTS NEW VERSION; *ref. in C.P.C.*: 2 (1971) 180.

*Author of original program*: A. Hibbert

*Computer*: ICL 1906A; *Installation*: Atlas Computer Laboratory, Chilton, Didcot, Berkshire, U.K.

*Operating system*: George 4

*Programming language used in adapted program*: FORTRAN IV

*High speed store required*: 28 Kwords.

*No. of bits in a word*: 24

*No. of cards required to effect adaptation (including directive cards)*: 225

*C.P.C. Library subprograms used*:

| *Catalogue number* | *Title* | *Ref. in C.P.C.* |
|---|---|---|
| ACQB | P SHELL CFP | 1(1969)15 |
| ACRN | A NEW D SHELL CFP | 6(1973)88 |
| AAGD[†] | NJSYM | 1(1970)241 |
| AAGD0001 | ADAPT NJSYM FOR WEIGHTS | 2(1971)180 |
| AAGD0002 | ADAPT TO INTEGER ARITHMETIC | 5(1973)161 |

*Purpose of adaptation*: to check the configuration input data for possible errors or inconsistencies.

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[†] Note that AAHD A NEW VERSION OF NJSYM [Computer Phys. Commun. 8 (1974) 149] can be used in the place of AAGD and these two adaptations.

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# ERRATUM NOTICE

*Title of manuscript*: Program for evaluation of non-exchange type integrals required in electron-atom scattering theory using Slater-type orbitals as basis functions.

*Authors*: Richard L. Smith and Donald G. Truhlar

*Reference*: Computer Phys. Commun. 5 (1973) 80

*Titles of programs*: NETI and NETIX

*Catalogue numbers*: AAGP and AAGT

*Computer on which corrected program was run*: Control Data Corporation CYBER 74

*Installation*: University Computer Center of the University of Minnesota

*High speed storage required by corrected program*: 9920 words (NETI) and 13888 words (NETIX)

*Typical running times for corrected NETI*:
Typical running times (CPU time) per $I$ integral with $k_1 \neq k_2$ are less than a millisecond to 0.2 sec if NBI $\neq 1$ and less than a millisecond to 0.01 sec if NBI = 1. The test run for the corrected program requires 6 sec (excluding compilation).

*Typical running times for corrected NETIX*:
The test run for the corrected program requires 31 sec (excluding compilation).

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 349–376. NORTH-HOLLAND PUBLISHING COMPANY

# EXACT FINITE RANGE DWBA CALCULATIONS FOR HEAVY-ION INDUCED NUCLEAR REACTIONS

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*Center for Nuclear Studies*, University of Texas, Austin, Texas 78712, USA*

Received 17 July 1974

## PROGRAM SUMMARY

*Title of program*: SATURN-1-FOR-EFR-DWBA

*Catalogue number*: ABPA

*Computer*: CDC 6600; *Installation*: Univ. of Texas Computation Center

*Operating system*: UT2D

*Programming language used*: FORTRAN IV

*High speed store required*: 32704 words

*Number of bits per word*: 60

*Overlay structure*: None

*Number of magnetic tapes required*: 3

*Other peripherals used*: Card reader, line printer, punch

*Number of cards in combined program and test deck*: 2509

*Keywords*: Nuclear, heavy ion, direct nuclear transfer reactions, exact finite-range DWBA (with recoil), no-recoil approximation, form factor, stripping, pickup, cross section, elastic scattering, Schrödinger equation, EFR–DWBA, NR–DWBA.

## PROGRAM SUMMARY

*Title of program*: MARS-1-FOR-EFR-DWBA

*Catalogue number*: ABPB

*Computer*: CDC 6600; *Installation*: Univ. of Texas Computation Center

*Operating system*: UT2D

*Programming language used*: FORTRAN IV

*High speed store required*: 29632 words

*Number of bits per word*: 60

*Overlay structure*: None

*Number of magnetic tapes required*: 3

*Other peripherals used*: Card reader, line printer

*Number of cards in combined program and test deck*: 2175

*Keywords*: Nuclear, heavy ion, direct nuclear transfer reactions, exact finite-range DWBA (with recoil), no-recoil approximation, form factor, stripping, pickup, cross section, elastic scattering, Schrödinger equation, EFR–DWBA, NR–DWBA.

*Nature of physical problem*
The package SATURN-MARS-1 consists of two programs SATURN and MARS for calculating cross sections of reactions transferring nucleon(s) primarily between two heavy ions. The calculations are made within the framework of the finite-range distorted wave Born approximation (DWBA). The first part, SATURN, prepares the form factor(s) either for exact finite-range (EFR) or for no-recoil (NR) approach. The prepared form factor is then used by the second part MARS to calculate either EFR–DWBA or NR–DWBA cross sections.

*Method of solution*
Either with EFR or NR approaches, a one-dimensional integral(s) is to be carried out in SATURN to evaluate certain kernel(s). There the gaussian quadrature is used, introducing

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* Supported in part by the US Atomic Energy Commission.

a specific technique [1] so as to minimize the number of quadrature points. Most of the basic techniques used in MARS are not very much different from those used in VENUS, a zero-range (ZR) DWBA program reported earlier [2]. Throughout SATURN and MARS, interpolation and other techniques [1] are used, so that EFR calculations can be performed with a speed which is not very much slower than the much simplified NR and/or ZR approximations.

*Restrictions on the complexity of the program*
In its present shape, SATURN-MARS-1 requires the use of the cluster approximation for treating multi-nucleon transfer reactions. Note, however, that in many applications the cluster approximation is sufficiently good, and also that removal of this restriction is made rather easily, by writing a booster program to feed results into SATURN. Presently set restrictions on the size of the calculations can be removed fairly easily without increasing the needed core very much.

*Typical running time*
The largest calculation so far made with SATURN-MARS-1 is the analysis of $^{208}$Pb($^{16}$O, $^{15}$N)$^{209}$Bi reactions with $E(^{16}\mathrm{O}) = 140$ MeV. With the CDC 6600 computer at the University of Texas, the running time ranged from 2 to 8 minutes when the spin of the final states in $^{209}$Bi varied from 1/2 to 9/2. With the IBM360/195 computer at the Argonne National Laboratory, the running time of the same calculation was about 1/3 of the above figure. When lighter targets and lower $E$ were used, most of the calculations were made within a minute, even with the CDC 6600.

*References*

[1] T. Tamura and K.S. Low, Phys. Rev. Letters 31 (1973) 1356;
K.S. Low and T. Tamura, Phys. Letters 48B (1974) 285;
T. Tamura, Phys. Rep., to be published.
[2] T. Tamura, F. Rybicki and W.R. Coker, Computer Phys. Commun. 2 (1971) 94.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 377–395. NORTH-HOLLAND PUBLISHING COMPANY

# COULOMB WAVE FUNCTIONS FOR ALL REAL $\eta$ AND $\rho$ [*]

A.R. BARNETT, D.H. FENG [**], J.W. STEED [‡] and L.J.B. GOLDFARB
*Physics Department, Schuster Laboratory, The University, Manchester M13 9PL, UK*

Received 25 July 1974

## PROGRAM SUMMARY

*Title of program*: RCWFN

*Catalogue number*: ABPC

| *Computer*: | *Installation*: |
|---|---|
| CDC 7600 | University of Manchester Regional Computing Centre |
| IBM 370/165 | Daresbury Nuclear Physics Laboratory, Warrington, Lancs. |
| IBM 360/195 | Rutherford High Energy Laboratory, Didcot, Berks. |

*Operating system*: UMRCC Scope V2.0

*Programming language used*: ASA Fortran

*High-speed core required*: < 1 Kwords

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in the combined program and test deck*: 282

*Keywords*: Nuclear, atomic, Schrodinger equation, reactions, scattering, heavy ion, wavefunction, Coulomb, potential, hypergeometric function, continued fraction, Runge–Kutta.

*Nature of the physical problem*
The subroutine RCWFN calculates the regular and irregular Coulomb wavefunctions, $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$ and their radial derivatives for real, positive energy for all $(\eta,\rho)$, $(-1000 \leqslant \eta \leqslant 1000, \rho > 0)$ rapidly and with high accuracy. It is well suited for calculations of Coulomb matrix elements for heavy-ion scattering [1] $(1 < \eta < 200, \eta < \rho < 1000)$ and for all programs which require matching to asymptotic Coulomb wavefunctions in both nuclear and atomic physics.

*Method of solution*
An entirely new technique, developed by Steed [2], is used, which differs greatly from standard methods [3]. The method is based on the continued-fraction expansion of the quantities $F_l'/F_l$ and $(G_l' + iF_l')/(G_l + iF_l)$ and it is applicable for all values of $\rho \geqslant \rho_{TP} = \eta + [\eta^2 + l(l+1)]^{1/2}$ without restriction. A somewhat modified method is used for values of $\rho < \rho_{TP}$. The results are given for all $l$-values between MINL and MAXL inclusive (MAXL $\geqslant$ MINL $\geqslant$ 0) and for any required $\rho$-value. In general results are obtained without integrating the differential equation. The subroutine is fast and compact [‡‡]; the results can be obtained to any desired accuracy in the range $10^{-6}$–$10^{-12}$.

*Restriction on the complexity of the problem*
Subroutine RCWFN has been programmed for real values of $\eta$ and $\rho$: the value of $\eta$ is unrestricted (positive, negative or zero) while the value of $\rho$ cannot be zero. There is a loss of accuracy in cases when $\rho < 0.2\rho_{TP}$.

*Typical running time*
For the $l = 0$ functions the averaging running time (CDC 7600 CP time) is 0.005 sec for ACCUR = $10^{-7}$ and STEP = 100.0 (i.e. practical values), and there is no significant increase with $l$-value.

*References*

[1] A.R. Barnett, D.H. Feng and L.J.B. Goldfarb, Phys. Lett. 48B (1974) 290; and Computer Phys. Commun., to be published.
[2] J.W. Steed, PhD thesis, University of Manchester (1967) unpublished.
[3] C.E. Froberg, Rev. Mod. Phys. 27 (1955) 399;
C. Bardin et al., Computer Phys. Commun. 3 (1972) 73.

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[*] Work supported by the United Kingdom Science Research Council.

[**] Present address: Center for Nuclear Studies, University of Texas, Texas, USA.

[‡] Now with Software Sciences Limited, Park Green, Macclesfield, UK.

[‡‡] When the $-separator format on the CDC card input is used the entire subroutine occupies 36 cards.

COMPUTER PHYSICS COMMUNICATIONS 8 (1974) 396–403. NORTH-HOLLAND PUBLISHING COMPANY

# BOUND STATES OF ONE NUCLEON IN A WOODS–SAXON WELL FROM A VARIATIONAL METHOD

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*Sart-Tilman, B-4000 Liège 1, Belgium*

and

Daniel M. DUBOIS
*Université de Liège, Institut de Mathématique,*
*15, Avenue des Tilleuls, B-4000 Liège, Belgium*

Received 13 August 1974

## PROGRAM SUMMARY

*Title of program*: OSCI

*Catalogue number*: ABMJ

*Computer*: IBM 370/158; *Installation*: University of Liege

*Operating system*: VS2-RO1.6

*Programming language used*: FORTRAN IV G1

*High speed store required*: 128 K bytes

*No. of bits in a byte*: 8

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 613

*Keywords*: Nuclear, bound states, Woods–Saxon, harmonic oscillator, Tobocman and Nagarajan, variational method.

*Nature of the physical problem*

The program computes the wave function characterized by an orbital angular momentum $L$ for the bound states with $J = L + \frac{1}{2}$ and $J = L - \frac{1}{2}$ of a particle in a Woods–Saxon potential with spin–orbit coupling.

*Method of solution*

The solution of the radial Schrödinger equation for a particle in a Woods–Saxon potential is developed on a complete set of orthonormal wave functions $\phi_{NL}$, solutions of the radial Schrödinger equation for the harmonic oscillator potential, in the framework of Tobocman and Nagarajan's variational method [1].

*Restrictions on the complexity of the problem*

This method was only used for neutral particles. The maximum number of harmonic oscillator wave functions (NMAX) is restricted to 10. The above restriction is easy to relax by small changes in the program.

*Reference*

[1] W. Tobocman and M.A. Nagarajan, Phys. Rev. 138 (1965) B1351.

Computer Physics Communications 9 (1975) 11–30
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# COCHASE, A CODE FOR COUPLED CHANNEL SCHRÖDINGER EQUATIONS *

S. HIRSCHI, E. LOMON and N. SPENCER
*Laboratory for Nuclear Science and Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

Received 3 June 1974

## PROGRAM SUMMARY

*Title of program*: COCHASE

*Catalogue number*: ABIC

*Computer*: IBM 360/65; *Installation*: Laboratory for Nuclear Science, M.I.T.

*Operating system*: OS 360 MFT/HASPII

*Programming language used*: FORTRAN IV

*High speed storage required*: 122 K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1358

*Keywords*: Nuclear, $S$-matrix, coupled channels, phase shift, inelasticity, Schrödinger equation, coupled differential equations, Runge–Kutta, Newton–Raphson.

*Nature of the physical problem*
The computer code COCHASE is designed to calculate the $S$-matrix in the form of a real phase shift and inelasticity for the interaction of two particles coupled to the possible production of five other two particle channels. The production cross section for each secondary channel is also easily obtained.

*Method of solution*
The method of solution is to solve a set of coupled differential Schrödinger equations for the wave functions in each channel using a fourth order Runge–Kutta routine. Two simultaneous transcendental equations which involve these wave functions are then solved using the Newton–Raphson technique to find the phase shift and inelasticity.

*Restrictions on the complexity of the problem*
The program is limited to the production of at most five two-particle channels. The potentials in the Schrödinger equations are assumed to be real and symmetric. Both of these restrictions are not essential and could be removed by some reprogramming.

Those channels which involve Coulomb potentials are energy restricted, since numerical expressions have been used for the Coulomb functions which define the wave functions at large distances. These expressions hold for large $\rho$ ($\rho = kx$). Since $x$ is approximately 10 fermi and $k$ is proportional to the energy, calculations below 10 MeV will be inaccurate. This restriction can be removed by using routines which have been written to calculate Coulomb functions in this region.

There is also a problem with maintaining accuracy on the phase shift and inelasticity (see Section 4) when far below inelastic thresholds. Double precision code is used for the test case.

*Typical running time*
The test case which involved the production of two two-particle channels at four energies took 2 min. of IBM 360/65 time to compile, link-edit and execute.

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* This work has been supported in part by the Atomic Energy Commission under Contract No. AT (11-1)-3069.

Computer Physics Communications 9 (1975) 31–45
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# A MULTICONFIGURATION RELATIVISTIC DIRAC–FOCK PROGRAM

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*Centre d'Etude de Limeil, B.P. 27, 94190 Villeneuve St. Georges, France*

Received 30 April 1974

## PROGRAM SUMMARY

*Title of program:* Multiconfiguration DIRAC–FOCK

*Catalogue number:* ACRV

*Computer:* IBM 370/155, DEC PDP10; *Installation:* C.E.L. Institut Laue–Langevin

*Operating system:* OS and HASP 3

*Programming language used:* FORTRAN IV

*High speed store required:* 348K bytes

*No. of bits in a byte:* 8

*Overlay structure:* None

*No. of magnetic tapes required:* zero to three

*Other peripherals used:* Card reader, card punch, printer

*No. of cards in combined program and test deck:* 4431

*Keywords:* Atomic structure, relativistic Dirac–Fock, configuration interaction, Dirac equation, wavefunctions, eigenvalues, predictor–corrector method, self-consistent field.

*Nature of the physical problem*
The relativistic Dirac–Fock equations, for neutral atoms or ions in a bound state, are solved numerically within the multiconfiguration approximation.

*Method of solution*
The two, first-order coupled Dirac equations are solved by a five-point, numerical, corrector–predictor method [1]. The "in–out" method described by Hartree [2] is used. Self consistency is obtained by an iterative process. All the one-electron functions are required to be orthogonal.

*Restrictions on the complexity of the problem*
The orthogonality constraint leads to off-diagonal Lagrange multipliers in the Dirac–Fock equations. There are difficulties to solve the equations in the special case of two open shells with the same symmetry and same occupation number. For this situation the multipliers have to be assumed to be zero but then, of course, the wavefunctions are only approximately orthogonal. The interactions between configurations are assumed to be expressed in terms of $F^k$, $G^k$ and $R^k$ integrals and this assumption precludes the consideration of single excited configurations which are coupled through one-electron operators.

*Unusual features of the program*
Three possibilities are provided for the proton charge distribution, namely: 1. point charge; 2. constant charge inside a sphere 3. Fermi distribution. An analytical approximation of the Thomas–Fermi potential is included in the program deck such that no initial wavefunctions are required to start the iterative process. Nevertheless, in certain cases the Thomas–Fermi potential may be such a poor initial approximation that convergence will not be achieved. In this case it is possible to use either hydrogenic or previously computed functions as initial estimates. As many orbitals as desired may be frozen.

*Typical running time*
The test case consisting of 1. Single configuration ground state of the lithium atom with a Fermi distribution for the nuclear charge; 2. Single configuration ground state of the neon atom with a constant proton charge distribution; 3. Ground state of the nitrogen atom (which involves three configurations in intermediate coupling) with a point charge nucleus; requires 160 seconds to compile and 270 seconds to run on the IBM 370/155.

*References*

[1] F.B. Hildebrand, *Introduction to numerical analysis* (McGraw Hill, New York, 1956).
[2] D.R. Hartree, *The calculation of atomic structure* (John Wiley, New York, 1957).

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* Present adress: Institut Laue–Langevin, B.P. 156, 38042 Grenoble, France.

Computer Physics Communications 9 (1975) 46–50
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# A SUBROUTINE AND PROCEDURE FOR THE RAPID CALCULATION OF SIMPLE OFF-DIAGONAL RATIONAL APPROXIMANTS

P.R. GRAVES-MORRIS and D.E. ROBERTS
*Mathematical Institute, University of Kent, Canterbury, Kent, UK*

Received 25 March 1974

## PROGRAM SUMMARY

*Title of program:* FORTRAN CALCULATION OF SODS

*Catalogue number:* ACRS

*Computer:* ICL 4130; *Installation:* University of Kent

*Operating system:* DES 2

*Programming language used:* FORTRAN IV

*High speed storage required:* 5000 words

*No. of bits in a word:* 24

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer

*No. of cards in combined program and test deck:* 343

*Reference to other published version of this program*
*Cat. no.:* ACRT; *Title:* ALGOL CALCULATION OF SODS; *Ref. in CPC:* 9 (1975) 46 (this paper).

*Keywords:* General, rational, approximant, Chisholm, simple off-diagonal, prong, perturbation series, Padé.

## PROGRAM SUMMARY

*Title of program:* ALGOL CALCULATION OF SODS

*Catalogue number:* ACRT

*Computer:* ICL 4130; *Installation:* University of Kent

*Operating system:* DES 2

*Programming language used:* ALGOL 60

*High speed storage required:* 5000 words

*No. of bits in a word:* 24

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer

*No. of cards in combined program and test deck:* 299

*Reference to other published version of this program*
*Cat. no.:* ACRS; *Title:* FORTRAN CALCULATION OF SODS; *Ref. in CPC:* 9 (1975) 46 (this paper).

*Keywords:* General, rational, approximant, Chisholm, simple off-diagonal, prong, perturbation series, Padé.

*Nature of physical problem*
These approximants may be applied for resummation of the perturbation series with two interaction hamiltonians, e.g., that in potential scattering given by the sum of an attractive and a repulsive Yukawa potential [1]; many other applications are envisaged, especially in the field of critical phenomena.

*Method of solution*
Prong methods [2,3]

*Restriction on complexity of problem*
The problem must be well-conditioned. Note that the programs are written for an ICL 4130 with 48 bits floating point word length.

*Typical running time*
$2N^4$ msec approximately

*Unusual features of program*
None

*References*

[1] P.R. Graves-Morris and C. Samwell, Kent preprint.
[2] R. Hughes Jones and G.J. Makinson, J. Inst. Maths. Applics. 13 (1974) 299.
[3] P.R. Graves-Morris, R. Hughes Jones and G.J. Makinson, J. Inst. Maths. Applics. 13 (1974) 311.

Computer Physics Communications 9 (1975) 51–58
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# OLYMPUS AND PREPROCESSOR PACKAGE FOR AN IBM 370/165

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*UKAEA Culham Laboratory, Abingdon, Berkshire, UK*

and

P.D. ROBERTS
*Ministry of Defence (PE), Aldermaston, Berkshire, UK*

Received 15 July 1974

## PROGRAM SUMMARY

*Title of program*: OLYMPUS FOR IBM 370/165

*Catalogue number*: ABUJ

*Computer*: IBM 370/165; *Installation*: AERE, Harwell, Didcot, Berks.

*Operating system*: HASP

*Programming language used*: FORTRAN

*High speed storage required*: 72K bytes

*No. of bits in a byte*: 8

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Disk, line printer

*No. of cards in combined program and test deck*: 2412

*Reference to other published version of this program*: *Catalogue number*: ABUF; *Title*: OLYMPUS; *Ref. in CPC*: 7 (1974) 245

*Keywords*: General purpose, preprocessor, control, utility, package, initial-value problems, simulation, computation, standard, framework, kernel.

*Nature of problem*
A standard methodology called the OLYMPUS system has been established for constructing, testing and operating Fortran programs which solve equations describing initial-value problems. A previously-published control and utility package [1] implements this system for the ICL 4/70, and the present package contains the corresponding version for IBM 360/370 series computers. It also includes a FORTRAN preprocessor which will insert labelled COMMON blocks int a source file using only one master copy of COMMON.

*Method of solution*
Ref. [1] should be consulted for the details of the OLYMPU system proper. The preprocessor reads the COMMON blocks into store on one channel NA, the source code on another channel NB, and outputs the expanded program as a data set on a third channel NC which is then passed to the compiler.

*Restrictions*
Different implementations of OLYMPUS are required for different types of computer to take account of differing word-lengths, channel numbers etc. The present package should work on most IBM 360 and 370 systems provided that the control cards are modified to suit local conventions. Since th preprocessor is written in Standard FORTRAN it can, in pri ciple, be used on any computer. However, it has been design to take advantage of the IBM scheme for concatenating data sets.

*Reference*

[1] J.P. Christiansen and K.V. Roberts, Computer Phys. Co mun. 7 (1974) 245.

Computer Physics Communications 9 (1975) 59–63
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# MONTE CARLO CALCULATION OF MULTIPLE SCATTERING EFFECTS IN THERMAL NEUTRON SCATTERING EXPERIMENTS: MODIFICATION TO SLAB GEOMETRY*

J.R.D. COPLEY‡
*Argonne National Laboratory, Argonne, Illinois 60439, USA*

Received 5 July 1973

## ADAPTATION SUMMARY

*Title of adaptation*: SLAB GEOMETRY

*Adaptation number*: 0001

*Reference to original program*:

*Catalogue number*: ACIC

*Title*: SLOW NEUTRON MULTIPLE SCATTERING

*Ref. in CPC*: 7 (1974) 289.

*Author of original program*: J.R.D. Copley

*No. of cards required to effect adaptation (including directive cards)*: 392

*Nature of physical problem*
This adaptation modifies "SLOW NEUTRON MULTIPLE SCATTERING" [1] to calculate multiple scattering effects in a plane slab target.

*Reference*

[1] J.R.D. Copley, Computer Phys. Commun. 7 (1974) 289.

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# MONTE CARLO CALCULATION OF MULTIPLE SCATTERING EFFECTS IN THERMAL NEUTRON SCATTERING EXPERIMENTS: MODIFICATION TO HORIZONTAL CYLINDER GEOMETRY*

J.R.D. COPLEY‡
*Argonne National Laboratory, Argonne, Illinois 60439, USA*

Received 5 July 1973

## ADAPTATION SUMMARY

*Title of adaptation*: HORIZONTAL CYLINDER GEOMETRY

*Adaptation number*: 0002

*Reference to original program*:

*Catalogue number*: ACIC

*Title*: SLOW NEUTRON MULTIPLE SCATTERING,

*Ref. in CPC*: 7 (1974) 289.

*Author of original program*: J.R.D. Copley

*No. of cards required to effect adaptation (including directive cards)*: 298

*Nature of physical problem*
This adaptation modifies "SLOW NEUTRON MULTIPLE SCATTERING" [1] to calculate multiple scattering effects in a target consisting of multiple cylinders, with axes parallel to the scattering plane.

*Reference*
[1] J.R.D. Copley, Computer Phys. Commun. 7 (1974) 289.

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* Based on work performed under the auspices of the U.S. Atomic Energy Commission.

‡ Present address: Institut Max von Laue – Paul Langevin, B.P. 156, 38042 Grenoble Cédex, France.

Computer Physics Communications 9 (1975) 85–91
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# A PLOTTING PACKAGE FOR VISUAL COMPARISON OF POINTS AND CURVES

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*Royal Holloway College, Egham Hill, Egham, Surrey, UK*

and

R.C. BECKWITH
*Centre for Computing and Automation, Imperial College, London, S.W.7, UK*

Received 21 June 1974

## PROGRAM SUMMARY

*Title of program:* APLOT

*Catalogue number:* AAUN

*Computers:* CDC 6600, CDC 7600; *Installation:* University of London Computer Centre.

*Operating system:* SCOPE

*Programming language used:* FORTRAN IV

*High speed core required:* 18Kwords

*No. of bits in a word:* 60

*Overlay structure:* None

*Number of magnetic tapes required:* None

*Other peripherals used:* Card reader, Calcomp plotter or plotter with Calcomp compatible software.

*Number of cards in combined program and test deck:* 1261

*Keywords:* General, graph, cartesian, log–linear, log–log, histogram.

*Nature of the physical problem*
This program is concerned with the visual display of theoretical and experimental results.

*Method of solution*
A sequence of subroutines is developed based on the Calcomp routines supplied by the University of London Computer Centre for plotting cartesian, log–linear, log–log graphs and histograms.

*Restrictions on the complexity of the program*
The only restriction on the program is the number of theoretical and experimental points to be plotted.

*Typical running time*
A recent application [1] reproduced here as the test run took about 10 seconds.

*References*

[1] P.A. Collins, B.J. Hartley, R.W. Moore and K.J.M. Moriarty, Nuclear Physics B20 (1970) 381.

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☆ Department of Statistics and Computer Science.
★ Department of Mathematics.

Computer Physics Communications 9 (1975) 92–101
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# PROGRAM FOR SPECTRA AND CROSS-SECTION CALCULATIONS WITHIN THE PRE-EQUILIBRIUM MODEL OF NUCLEAR REACTIONS

Emil BĚTÁK
*Institute of Physics, Slovak Academy of Sciences, Dúbravská cesta, 899 30 Bratislava, Czechoslovakia*

Received 20 August 1974

## PROGRAM SUMMARY

*Title of program:* PREEQ

*Catalogue number:* ABGO

| *Computer:* | *Installation:* |
|---|---|
| CDC 3300 | Comp. Res. Ctr. U.N.D.P. Bratislava, Czechoslovakia |
| SIEMENS 4004/50 | Univ. Inst. Comp. Technique, Bratislava, Czechoslovakia |

*Operating system:* MASTER 3

*Programming language used:* FORTRAN IV

*High speed storage required:* 20,992 words

*No. of bits in a word:* 24 but real variable is stored in two words.

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer

*No. of cards in combined program and test deck:* 816

*Keywords:* Nuclear, reactions, pre-equilibrium, decay, exciton model, master-equation approach, iteration, complex particles, energy spectra.

*Nature of physical problem*
The program calculates particles spectra and/or cross-sections within the pre-equilibrium model of nuclear reactions using the master-equation approach to the model. The complex particles and the competition among various channels are also included in the calculation.

*Method of solution*
In the first part of the program, the emission rates for all outgoing channels and the transition rates are calculated. They enter the set of master equations describing the equilibration process and the decay. This set is solved by an iteration and after reaching the equilibrium its solution is extrapolated in time to infinity. Finally, the desired particle spectra and/or cross-sections are calculated.

*Restrictions on the complexity of the problem*
The complex particle emission may be calculated, but the successive particle emission is not included in the program. The maximum energy of the outgoing particles is restricted to 100 MeV. The composite nucleus can be created only by particles with mass numbers not exceeding 4.
The program supposes that 4 alphanumeric characters can be stored in one integer variable place. If not, minor modifications are required in the program. The commands, which may require to be changed, are flagged by a comment.

*Typical running time*
The running time depends on the composite nucleus energy and the number of open (or desired) reaction channels. For the excitation energy of 50 MeV and the maximum, i.e. 6 outgoing particles, the running time is about 1 minute for the CDC 3300 computer.
For repeated calculations with slightly changed parameters part of the previous results is used, if possible, so that the necessary time is reduced.

Computer Physics Communications 9 (1975) 102–116
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# A GENERAL PROGRAM TO CALCULATE THE MATRIX OF THE SPIN–ORBIT INTERACTION

W.-D. KLOTZ
*Technische Universitaet Berlin, Institut für Strahlungs und Kernphysik, 1000 Berlin 37, Rondellstrasse 5, Germany*

Received 4 June 1974

## PROGRAM SUMMARY

*Title of program*: SPINORBIT WEIGHTS

*Catalogue number*: AAKL

*Computer*: CDC 6600; *Installation*: Technical Univ. Berlin, Germany

*Operating system or monitor under which the program is executed*: Scope 3.4

*Programming language used*: Fortran

*High speed storage required*: 26278 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1549

*CPC Library subprograms used*:

| *Catal. no.*: | *Title*: | *Ref. in CPC*: |
|---|---|---|
| ACQB | CFPP | 1 (1969) 15 |
| ACQC | CFPD | 1 (1969) 16 |
| AAGD | NJSYM | 1 (1970) 241 |

*Keywords*: Atomic, structure, fine structure, hyper-fine structure, configuration interaction, complex atoms, wave function, spin–orbit coupling, *LS*-coupling, recoupling, Racah, tensor operator, *Nj*-symbols, coefficients of fractional parentage.

*Nature of physical problem*
In atomic structure calculations with configuration interaction, one has to evaluate the matrix of the hamiltonian with respect to a basis set of configuration wave functions. For configurations with several open shells, the calculation of the matrix elements becomes cumbersome. A general program, which calculates the two-body part of the hamiltonian, exists already [1]. We present a program which calculates the one-body spin–orbit interaction.

*Method of solution*
The coefficients of the spin–orbit radial integrals are obtained by integration over the coordinates of $N-1$ spectator electrons and the angular coordinates of the interacting electron of an $N$-electron atom. We used the scheme of Fano [2] in analogy to a one-particle operator, using techniques of Racah [3] and Briggs [4]. We modified the program of Hibbert [1] and used some of his subroutines. The coefficients are expressed as sums over cfp-coefficients [5], recoupling coefficients [6] and reduced matrix elements [7, 8]. The configurations are defined by their occupied *nl*-shells and their numbers of electrons. The coupling schemes are defined by the $S,L$-values of the shells and their intermediate couplings.

*Restrictions on the complexity of the problem*
Only configurations with any number of electrons in s-, p- and d-shells are allowed, but no more than two electrons in any shell of higher orbital momentum. The submitted version allows up to 3 different configurations, 10 occupied shells and 60 coupling schemes in each configuration.

*Typical running time*
The running time of the test run is 8.2 sec on a CDC 6600 during which 64 matrix elements are calculated.

*Unusual features*
A punch option is provided, but a punch subroutine has to be written by the user according to his individual problems.

*References*

[1] A. Hibbert, Computer Phys. Commun. 1 (1969) 359 and 2 (1971) 180.
[2] U. Fano, Phys. Rev. 140, 1A (1965) A67.
[3] G. Racah, Phys. Rev. 63 (1943) 367.
[4] J.S. Briggs, J. Math. Phys. 11, 4 (1970) 1198.
[5] D.C.S. Allison, Computer. Phys. Commun. 1 (1969) 15.
[6] P.G. Burke, Computer. Phys. Commun. 1 (1970) 241.
[7] A.R. Edmonds, Angular Momentum in Quantum Mechanics (Princeton Univ. Press, 1960).
[8] S. Feneuille, J. Phys. Radium 28 (1967) 61.

Computer Physics Communications 9 (1975) 117–128
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# A LEAST-SQUARES SPECTRAL CURVE FITTING ROUTINE FOR STRONGLY OVERLAPPING LORENTZIANS OR GAUSSIANS

E. von MEERWALL
*The University of Akron, Akron, Ohio 44325, USA*

Received 14 October 1974

## PROGRAM SUMMARY

*Title of program*: LGFIT2

*Catalogue number*: ABMK

*Computer*: IBM 370/155; *Installation*: The University of Akron, Akron, Ohio, USA.

*Operating system*: OS/MVT

*Programming langauge used*: FORTRAN IV(G)

*High speed store required*: 34,000 words (135 kbt)

*Number of bits in a word*: 32

*Overlay structure*: None

*Number of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, Calcomp incremental plotter (optional).

*Number of cards in combined program and test deck*: 1366

*Keywords*: Nuclear, gamma ray, magnetic, resonance, Mössbauer effect, spectroscopy, least squares fit, non-linear, variable metric, iterative solution, constraint.

*Nature of physical problem*

A program is described for fitting a background level plus or minus the sum of a number of lorentzian or gaussian lineshapes to experimental spectra, honoring linear constraints between arbitrary pairs of parameters.

*Method of solution*

A non-linear variable metric minimization technique [1] is used iteratively to optimize the parameters of the theoretical function by minimizing $\chi^2$ for the spectral data.

*Restrictions on program complexity*

Present dimensions of the program permit a maximum number of 512 spectral data points and a maximum of 49 adjustable parameters (16 peaks and background). These limits may be changed by redimensioning, and altering several preliminary check statements.

*Typical running time*

On the IBM 370/155 at The University of Akron, the program compiles in about 20 CPU seconds. A fit of less than ten parameters to a 60-point spectrum, with plotting, takes about 6 seconds. A fit of 13 lorentzian lines (40 parameters) with 17 constraints, to 256 points, testing the optimal fit by refitting after each of three random parameter displacements, and plotting output on the line printer and the Calcomp plotter, took 80 seconds CPU time.

*Unusual features of the program*

The program is intended to give general fitting capabilities for resonance spectroscopy of various kinds, particularly Mössbauer, nuclear gamma ray, and nuclear magnetic resonance spectroscopy. Therefore, several unorthodox features have been implemented:

1. The program accepts spectral data of the general form $(x_i, y_i, w_i)$, where $x_i$ may be unequally spaced, and $w$ is the weight of the data point; $w_i \equiv (\Delta y_i)^{-2}$, for example. For multichannel counting spectra, input of $x$ and $w$ may be suppressed. A desired number of points contributing most to $\chi^2$ may be dropped ($w \to 0$) after the first fitting cycle.
2. Linear constraints between pairs of parameters to the optimized may be implemented, and released after a selected number of fitting cycles.
3. The spectral preprocessor may be instructed to integrate the (derivative) spectrum prior to the fit, e.g., for wide-line NMR use. Suitable background adjustment may be selected from several options. For Mössbauer effect use, the data may be corrected for parabolic baseline curvature.

*Reference*

[1] W. Davidon, U.S. AEC Research and Development Report ANL-5990, 1959 (Appendix).

Computer Physics Communications 9 (1975) 129
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# ERRATUM NOTICE

*Title of manuscript*: Relativistic self-consistent field program for atoms and ions.

*Authors*: D.A. Liberman, D.T. Cromer and J.T. Waber

*Reference*: Computer Physics Communications 2 (1971) 107.
*Title of program*: HEX
*Catalogue number*: AAKB

Computer Physics Communications 9 (1975) 141–172
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# CIV3 – A GENERAL PROGRAM TO CALCULATE CONFIGURATION INTERACTION WAVE FUNCTIONS AND ELECTRIC-DIPOLE OSCILLATOR STRENGTHS

A. HIBBERT
*Department of Applied Mathematics & Theoretical Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland*

Received 28 August 1974

## PROGRAM SUMMARY

*Title of program*: CIV3 A GENERAL C.I. PROGRAM

*Catalogue number*: AAKM

*Computer*: ICL 1906A; *Installation*: Atlas Computer Laboratory, Chilton, Didcot, Berks., U.K.

*Operating system*: George 4

*Programming language used*: FORTRAN IV

*High speed storage required*: 57K words

*No. of bits in a word*: 24

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer; plus card punch and second card reader channel (both optional)

*No. of cards in combined program and test deck*: 5583

*C.P.C. Library subprograms used*:

| *Cat. numbers* | *Titles* | *Refs. in C.P.C.* |
|---|---|---|
| ACQB | P SHELL C.F.P. | 1 (1969) 15 |
| ACRN | A NEW D SHELL C.F.P. | 6 (1973) 88 |
| AAGD | NJSYM | 1 (1970) 241 |
| AAGD0001 | ADAPT NJSYM FOR WEIGHTS | 2 (1971) 180 |
| AAGD0002 | ADAPT TO INTEGER ARITHMETIC | 5 (1973) 161 |
| ACQV | WEIGHTS NEW VERSION | 2 (1971) 180 |
| ACQV0001 | ADAPT WEIGHTS FOR ONE-ELECT | 7 (1974) 318 |
| ACQV0002 | ADAPT TO TEST CONFIG DATA | 8 (1974) 329 |
| AAKF | REDUCED TENSOR MATRIX ELEMENTS | 6 (1973) 132 |

*Keywords*: Atomic, configuration interaction, superposition of configurations, Racah, coefficients of fractional parentage, recoupling coefficients, Slater integrals, average energy, complex atoms, wave functions, bound states, $L-S$ coupling, nonlinear optimization, Slater-type orbitals, electric dipole matrix elements, transition probabilities, oscillator strengths.

*Nature of physical problem*
The program generates configuration interaction wave functions, which may then be used to calculate oscillator strengths of transitions in atomic systems.

*Method of solution*
(i) The hamiltonian matrix is set up; the angular integrals are performed using Racah algebra by the package ACQV [1] and those called by it; since the radial functions are expressed as sums of Slater-type orbitals, the radial integrals are performed analytically.
(ii) The hamiltonian matrix is diagonalized to obtain upper bounds to the exact energies (eigenvalues) and the components of the configurations in the corresponding wave functions (eigenvectors).
(iii) The parameters of one or more radial functions may be varied using an eigenvalue (or appropriate combination of eigenvalues) as the functional to be minimized.
(iv) Further configurations may be included, in order to define C.I. wave functions for two or more states. Oscillator strengths of transitions between states may be calculated.
(v) Similar calculations may then be performed for smaller sets of configurations, or for different members of an isoelectronic sequence.

*Restrictions on the complexity of the program*

The program assumes $L-S$ coupling throughout. The radial functions are analytic, although the number of basis functions allowed is limited only by the current dimensions of arrays. For a given $l$, the radial functions $\{P_{nl}\}$ form an orthonormal set. When several states are calculated in one run, the program assumes that the radial function $P_{nl}$ is the same for all states in which it is involved. In particular, since two states are involved in the evaluation of oscillator strengths, the wave functions used (or calculated) by this program must be constructed from a common set of radial functions.

Current dimension limits are described in §7 of the Long Write-up. With the present dimensions, correlation effects may be studied on atomic systems with up to about 12 electrons. The angular momentum package [1] called by this code allows up to the maximum number of electrons in s, p, d subshells, but only up to two electrons in f or g subshells, nor are subshells with $l > 4$ allowed without adaptations to [1].

*Typical running time*

Execution time depends on

(i) the size of the atom,
(ii) the extent of the optimization required,
(iii) the number of configurations involved,
(iv) the number of basis functions in each radial function.

The first case in the test run – to set up and diagonalize the hamiltonian matrix for 11 configurations of oxygen – took 55 seconds.

This program has about the same execution time on an ICL 1906A as on an IBM 360/75, and is about three times quicker on a CDC 6600.

*Reference*

[1] A. Hibbert, Computer Phys. Commun. 2 (1971) 180.

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Computer Physics Communications 9 (1975) 173–181
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# EXACT COMPUTATION OF THE ZEEMAN EFFECT ON NUCLEAR QUADRUPOLE RESONANCE PROFILES FOR POWDERS (SPIN $I = 3/2$). DETERMINATION OF THE ASYMMETRY PARAMETER

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Received 20 September 1974

## PROGRAM SUMMARY

*Title of program*: ASYMMETRY PARAMETER IN NQR

*Catalogue number*: ACKH

*Computer*: IBM 370/158; *Installation*: CECTI, University of Liege

*Operating system*: ASP/VS2 - RO1.6

*Programming language used*: FORTRAN IV

*High speed store required*: 28,000 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1350

*Keywords*: Solid state, asymmetry parameter, nuclear quadrupole resonance, powder simulation, Morino–Toyama method, convolution, line shape simulation, Zeeman effect.

*Nature of physical problem*
The asymmetry parameter ($\eta$) of the electric-field gradient tensor is to be determined precisely, using powder samples. The shape of the Zeeman effect envelope reflects a typical structure due to $\eta$.

*Method of solution*
The complete quadrupolar and Zeeman hamiltonian is treated exactly. Gaussian, lorentzian or "experimental line" convolution of the Dirac profile, followed by derivation, gives the first derivative envelope shape, to be compared to experimental results [1].

*Restrictions on the complexity of the problem*
The present version of the program is dimensioned so that 322 crystallites are considered to represent the powder. The total number of frequencies involved is then 1932 and 1288 are left in the interesting zone. The variables CO and DER are overdimensioned (1000). In fact their dimension would be in any case AKI plus the number of sampling points on the convolution function, where (AKI + 1) is the number of defining points for the interesting frequency zone. If the convolution function is the integrated experimental line, 2*NEXP+1 must be the number of sampling points.

*Typical running time*
On the IBM 370/158 of the University of Liege, the loading and assembly of the program and the collection of subroutines takes about 21 sec. The execution time is highly dependent on various factors, such as the number of values for the asymmetry parameter, the value of AKI and the number of crystallites (NCOUPL). To give a precise example (only one value of $\eta$), for a gaussian type convolution, AKI was chosen as 200. As deduced from the half-height width of the gaussian line, the number of sampling points on this one was equal to 25 and the computation time was then 70 sec.

*Unusual features of the program*
For the $\theta$ and $\varphi$ angles, increments of 2 and 15° respectively are chosen, in 1/8 of the sphere. More extended range of variations (0 to 180 degrees, for instance) has been proved unnecessary giving the same envelope shape as in the previous case. But the computation time is multiplied by a factor of about 4.

*References*

[1] J. Darville, A. Gérard and M.T. Calende, J. Magn. Resonance 16 (1974) 205.

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* Aspirant au F.N.R.S. (Bruxelles, Belgium).

Computer Physics Communications 9 (1975) 182–192
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# MONTE CARLO SIMULATION OF THE DIFFRACTIVE EXCITATION MODEL

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Received 4 February 1974

## PROGRAM SUMMARY

*Title of program*: DEM

*Catalogue number*: ABCK

*Computer*: IBM 360/195; *Installation*: Rutherford Lab., Didcot, UK

*Operating system*: MVT Rel. 21 HASP Version 3.1

*Programming language used*: FORTRAN IV

*High speed storage required*: 48K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Line printer

*No. of cards in combined program and test deck*: 689

*CPC Library subprograms used*: None

*Keywords*: Nuclear, high energy, elementary particles, multiparticle production, diffractive excitation, proton, nova, Monte Carlo simulation.

*Nature of physical problem*
The diffractive excitation model for multiparticle production in proton-proton collisions provides a framework for the calculation of experimentally observable distributions [1], both inclusive and exclusive. The dynamics occurs in two steps:
(1) excitation of the proton into a massive cluster
(2) de-excitation of the diffractive cluster by the subsequent emission of pions.
Events are characterized by the 4-momenta of two nucleons and the decay pions.

*Method of solution*
Importance sampling techniques are used in the Monte Carlo simulation of a random event. The events may be analyzed exactly like those from an experimental data summary tape.

*Restrictions on the complexity of the problem*
Only pions are produced, with an upper limit of 200 pions per cluster.

*Typical running time*
$1.7 \times 10^{-3}$ sec/event at $p_{\mathrm{INC}} = 30$ GeV/$c$, $1.0 \times 10^{-2}$ sec/event at $p_{\mathrm{INC}} = 1100$ GeV/$c$.

*Unusual features of the program*
All events respect exact kinematic constraints, being generated from tree diagrams, as in the CERN phase-space routine FOWL [2]. Events must be used in sets, each consisting of a fixed number (NUMB) of decay events.

*References*

[1] J. Kasman, The Diffractive Excitation Model for Multiparticle Production in Proton-Proton Collisions, Westfield College (London) preprint (April 1973).
[2] F. James, FOWL-A General Monte-Carlo Space Program, CERN program library W505 (1970).

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Computer Physics Communications 9 (1975) 193–204
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# A FINITE ELEMENT PROGRAM PACKAGE FOR AXISYMMETRIC VECTOR FIELD PROBLEMS

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Received 8 May 1974

## PROGRAM SUMMARY

*Title of program:* AXISYMM-VECTOR-HELMHOLTZ-FINTEL 6

*Catalogue number:* ACSE

*Computer:* IBM 360/75, IBM 370/158: *Installation:* McGill University Computing Centre, Montreal, Canada

*Operating system:* OS/360 with HASP-II

*Programming langauge used:* FORTRAN IV

*High speed storage required:* 50K words
*No. of bits in a word:* 32

*Overlay structure:* Overlaid

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer, card punch (optional)

*No. of cards in combined program and test deck:* 4463

*CPC Library subprograms used:*

| *Cat. number* | *Tittle* | *Ref. in CPC* |
|---|---|---|
| ACSC | AXISYMM-SCALAR-HELMHOLTZ-FINTEL 6 | 5(1973)438 |
| ACSF | VECTR FINTEL 6-BLK-DATA-GENERATOR | 9(1975)193 (this paper) |

*Keywords:* Plasma physics, fluid dynamics, magneto-hydrodynamics, Laplace, Poisson, Helmholtz, Bessel, axisymmetric, vector field, finite element, electrostatics, electromagnetics, electron optics, linear accelarator cavities, heat transfer.

*Nature of physical problem*
The following types of problems can be solved with the program:

– electromagnetic field problems requiring solution to the one-component vector Poisson or Helmholtz equation in cylindrical coordinates with no azimuthal variation (e.g. transformer problems, unsaturated magnetic lens problems, linear accelerator cavities);

– electric field problems requiring azimuthally periodic solutions to the scalar Laplace, Poisson or Helmholtz equation (i.e. solutions to the generalized Bessel equation of order $m$);

– a host of mathematically related problems which fall in the above two categories (e.g. heat and fluid flow problems).

*Method of solution*
The generalized Bessel equation of order $m$, derivable from the vector Helmholtz equation for $m = 1$ under the assumption of one vector component in the azimuthal direction and no azimuthal variation, or derivable from the scalar Helmholtz equation under the assumption of azimuthal periodicity, is solved by the high-order polynomial triangular finite-element method [1] using an approximation technique which avoids singularities of the $1/r$ type at the axis of symmetry.

*Restrictions on the complexity of the program*
Since the AXISYMM-VECTOR-HELMHOLTZ-FINTEL 6 program is closely modelled after the previously published scalar finite element programs [2], the same restrictions apply. The computations, as in the scalar case, are carried out in single precision arithmetic. For large problems round-off errors may accumulate during the solution of the matrix eigenvalue equation. This of course depends on the word length of the computer used.

*Typical running times*
The running times are similar to those cited in ref. [2] and can be estimated from the running times of the matrix equation solving subroutines.

*Unusual features of the program*
Most program features closely resemble those of the scalar programs [2].

Since computers other than the IBM 360 and 370 series may not accept the block data subprograms supplied with the program, a FORTRAN program (VECTR-FINTEL 6-BLK-DATA-GENERATOR) which punches out the complete block data subprograms is made available to the users.

*References*

[1] A. Konrad and P. Silvester, Int. J. Numer. Meth. Eng. 7 (1973) 43–55.
[2] A. Konrad and P. Silvester, Computer Phys. Commun. 5 (1973) 437–455.

## PROGRAM SUMMARY

*Title of program:* VECTR-FINTEL 6-BLK-DATA-GENERATOR

*Catalogue number:* ACSF

*Computer:* IBM 360/75, IBM 370/158; *Installation:* McGill University Computing Centre, Montreal, Canada

*Operating system:* OS/360 with HASP-II

*Programming language used:* FORTRAN IV

*High speed storage required:* 25 K words;
*No. of bits in a word:* 32

*Overlay structure:* None

*No. of magnetic tapes required:* None

*Other peripherals used:* Card reader, line printer, card punch

*No. of cards in combined program and test deck:* 1629

*Purpose of the program*
This program reads in the finite element matrices described in ref. [1] in integer form and punches out five complete block data subprograms containing these matrices in Z-format. The latter is an IBM Fortran IV feature which is convenient for compressing vast amount of numerical data. Users of the AXISYMM-VECTOR-HELMHOLTZ-FINTEL 6 finite element program (CPC catalogue number ACSE) who are using computers other than the IBM 360 or 370 series, will have to modify VECTR-FINTEL 6-BLK-DATA-GENERATOR in order to produce block data compatible with their Fortran IV compiler.

The test run output is the BLOCK DATA segments incorporated in AXISYMM-VECTOR-HELMHOLTZ-FINTEL 6.

*Typical running times*
It takes 25 seconds (CPU) on the IBM 360/75 computer to compile and execute VECTR-FINTEL 6-BLK-DATA-GENERATOR.

*References*

[1] A. Konrad and P. Silvester, Int. J. Numer. Meth. Eng. 7 (1973) 43–55.

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Computer Physics Communications 9 (1975) 231–246
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# NUMERICAL CALCULATIONS OF THE IRREDUCIBLE REPRESENTATIONS OF SPACE GROUPS

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*Via G. Capponi 9, 50121 Firenze, Italy*

Received 12 October 1974

## PROGRAM SUMMARY

*Title of program*: SPACE GROUP REPRESENTATIONS

*Catalogue number*: ACUA

| *Computer*: | *Installation*: |
|---|---|
| CII 10070<br>CDC6600 | Università di Firenze |

*Operating system*: SIRIS 7

*Programming language used*: FORTRAN IV

*High speed storage required*: 46000 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Printer, card reader, punch (optional)

*No. of cards in combined program and test deck*: 2124

*Keywords*: Solid state, group theory, space groups, symmetry, irreducible representations

*Nature of the physical problem*

The program computes the irreducible representations of any space group of $\boldsymbol{k}$, $G(\boldsymbol{k})$ [1], where $\boldsymbol{k}$ is a wave vector in the first Brillouin zone. For each irreducible representation of $G(\boldsymbol{k})$ a set of matrices, one for each space group coset representative, is obtained. No particular choice of origin of the coordinate system in a space group $G$ is required.

*Method of solution*

A definition of 1 up to 3 generators of the space group $G$ is used to obtain the multiplication properties of all coset representatives in $G$. An induction method is applied to compute the irreducible representations of $G(\boldsymbol{k})$ [2]. Herring's criterion provides a check for the existence of extra degeneracy due to time-reversal symmetry.

*Restrictions on the complexity of the problem*

This program is dimensioned for any space group, symmorphic or non-symmorphic, and for any value of $\boldsymbol{k}$ in the first Brillouin zone. No restriction is placed on the choice of the origin of the coordinate system in the space group. Complex algebra is used and matrix elements for the irreducible representations are obtained as complex numbers.

*Typical running time*

0.68 minutes were necessary for computing the irreducible representations of the space group $T_h^6$ (Pa3) for 14 different high-symmetry wave vectors.

*Unusual features of the program*

The irreducible representations, and the corresponding character tables, are printed out in symbolic form and symbols for point group elements are identified by maximally four alphanumeric characters, closely related to the usual Schoenflies notation.

*References*

[1] C.J. Bradley and A.P. Cracknell, The mathematical theory of symmetry in solids (Clarendon Press, Oxford, 1972).
[2] N. Neto, Acta Cryst. A29 (1973) 464.

Computer Physics Communications 9 (1975) 247–257
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# ILTHII – ANALYSIS OF THE SPECTRUM OF A THERMAL RADIOASTRONOMICAL SOURCE

M. SALEM

*Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK*

Received 4 September 1974

## PROGRAM SUMMARY

*Title of program*: ILTHII

*Catalogue number*: AAEF

*Computer*: IBM 360/65; *Installation*: University College London Computer Centre

*Operating system*: OS

*Programming language used*: FORTRAN IV

*High speed storage required*: 24000 words.

*No. of bits in a word*: 32

*Overlay structure*: Overlaid (29000 words required if not overlaid)

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, card punch (optional)

*No. of cards in combined program and test deck*: 4016

*Keywords*: Astrophysics, radioastronomy, HII region, thermal source, Laplace transform, inverse, continuum spectrum, minimization.

*Nature of physical problem*

It has been shown by Salem and Seaton [1] that, given the spectrum of a thermal radioastronomical source, information on the structure can be deduced in the form of a function $\Omega(E)$, which is the total angular area within which the emission measure is greater than or equal to $E$. A spherical model of the object can also be constructed [2]. An estimate of the electron temperature, $T_e$, (assumed to be constant) is required. In some cases this estimate may be improved by comparing $\Omega(E)$ with observations of high angular resolution. The computer program ILTHII (Inverse Laplace Transform – HII region) computes $\Omega(E)$ and the spherical model from the flux density spectrum, and also compares $\Omega(E)$ with high-resolution observations.

*Method of solution*

Observations of the flux density, $S_\nu$, as a function of frequency, $\nu$, are transformed to the form $y(x)$, where $x$ is essentially a frequency variable, and $y$ depends upon $S_\nu$ and $\nu$. An analytic function is fitted numerically to the observations; the inverse Laplace transform of this function is $[T_e\, \Omega(E)]$. An improved estimate of $T_e$ can, in principle, be made by adjusting $\Omega(E)$ to agree with high angular resolution observations.
If spherical symmetry is assumed, the electron density, $N_e$, can be determined as a function of distance from the center by analytical solution of an integral equation.

*Restrictions on the complexity of the problem*

The function $\Omega(E)$ is determined on the assumption that all continuum radio emission from the object is thermal, and that the electron temperature is essentially constant.

*Typical running time*

The running time depends upon the number of observations, the number of coefficients which define the function which fits the observations, and other user-specified quantities. The example provided took approximately 20 seconds to compile (excluding the minimization program), and 20 seconds to run on an IBM 360/65.

*References*

[1] M. Salem and M.J. Seaton, Mon. Not. R. astr. Soc. 167 (1974) 493.
[2] M. Salem, Mon. Not. R. astr. Soc. 167 (1974) 511.

Computer Physics Communications 9 (1975) 258–267
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# COMPUTATION OF LINE AND CONTINUUM RADIATION FROM THERMAL RADIOASTRONOMICAL SOURCES

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*Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK*

Received 4 September 1974

## PROGRAM SUMMARY

*Title of program:* RCMBLN

*Catalogue number:* AAEG

*Computer:* IBM 360/65; *Installation:* University College London Computer Centre.

*Operating system:* OS

*Programming language used*: FORTRAN IV

*High speed storage required*: 25000 words

*No. of bits in a word:* 32

*Overlay structure*: None

*No. of magnetic tapes required*: 2 (optional)

*Other peripherals used*: Card reader, line printer, card punch, (optional) disk(s).

*No. of cards in combined program and test deck*: 1239

*CPC Library subprograms used*: *Catalogue number*: AAEH; *Title*: SELECT BN, CN VALUES; *Ref. in CPC*: This paper.

*Keywords*: Astrophysics, radioastronomy, HII region, thermal source, radio recombination line, continuum spectrum.

*Nature of physical problem*

The interpretation of radio recombination lines is of importance to radio astronomy. The computer program described in this paper calculates the intensities and profiles of hydrogen and helium radio recombination lines emitted by a thermal source. The electron temperature is assumed to be constant throughout the source, while the electron density is a known function of position. Spherical or plane parallel symmetry is assumed in the program. The theory of the method used is described in detail by Brocklehurst and Seaton [1]. The construction of a spherical model of a thermal radio source, given the radio flux density spectrum, has been described by Salem and Seaton [2] and Salem [3], and a computer program which carries out the model construction has been written [4]. The model produced can be used as input to the present program.

*Method of solution*

Atomic hydrogen energy level populations have been computed by Brocklehurst [5] for different values of electron temperature, $T_e$, and electron density, $N_e$, in the form of coefficients of departure from thermodynamic equilibrium, $b_n$. As the coefficients of absorption and emission depend upon the $b_n$ factors, the equation of radiative transfer can be solved numerically for any given distribution of $T_e$ and $N_e$.

*Restrictions on the complexity of the problem*

The electron temperature is assumed to be constant throughout the source, and clumping is not taken into account. The equation of radiative transfer has been linearized by assuming that, for all lines, the optical depth due to line absorption (positive or negative) is much less, in absolute value, than unity; and that the line emissivity is much less than the continuum emissivity at the same frequency. These assumptions are adequate to within the accuracy of present day observations.

*Typical running time*

The running time depends greatly upon the number of points at which $N_e$ is specified. For 33 points, the running time is of the order of 2 seconds per line for a spherical model on an IBM 360/65 computer. Compilation time is approximately 20 seconds.

*References*

[1] M. Brocklehurst and M.J. Seaton, Mon. Not. R. Astr. Soc. 157 (1972) 179.
[2] M. Salem and M.J. Seaton, Mon. Not. R. Astr. Soc. 167 (1974) 493.
[3] M. Salem, Mon. Not. R. Astr. Soc. 167 (1974) 511.
[4] M. Salem, Computer Phys. Commun. 9 (1975) 247.
[5] M. Brocklehurst, Mon. Not. R. Astr. Soc. 148 (1970) 417.

## PROGRAM SUMMARY

*Title of program*: SELECT BN, CN VALUES

*Catalogue number*: AAEH

*Computer*: IBM 360/65; *Installation*: University Collge London Computer Centre.

*Operating system*: OS

*Programming language used*: FORTRAN IV

*High speed storage required*: 5,000 words.

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: 2 (optional)

*Other peripherals used*: Card reader. line printer, card punch (optional), up to 2 disks in place of tapes

*No. of cards in combined program and test deck*: 3864

*Keywords*: Astrophysics, radioastronomy, radio recombination line, $b_n$ values.

*Nature of physical problem*

The departure coefficients from thermodynamic equilibrium, $b_n$, and their derivatives, $c_n$, are required for the computation of intensities and profiles of hydrogen recombination lines from thermal radioastronomical sources. These coefficients have been computed by Brocklehurst [1] for values of $n$ up to 300, for 6 values of electron temperature, and for 8 values of electron density. As it is not expected that intensity calculations will be required for more than a few lines at a time, and as the information available is very extensive, a short program has been written to extract $b_n$ and $c_n$ values for up to 15 lines from the complete table, and to write them on a card, disk, or tape dataset in a form which can be read directly by program RCMBLN

*Restrictions on the complexity of the problem*

The program has been designed specifically to select $b_n$ and $c_n$ values from a table of fixed format. The table provided with the program corresponds to case B (radiation due to transitions to the ground state is reabsorbed; all other radiation escapes freely). Other similar tables can be substituted; in particular Brocklehurst [1] has also computed $b_n$ coefficients for case A (all radiation escapes freely).

*Typical running time*

The sample program took 3 seconds of CPU time to compile and 22 seconds to execute on an IBM 360/65 computer.

*Unusual features of the program*

The user may specify input and output units by means of a data card. He may also choose to read a table of values of the Voigt function, which will be written on the same output unit as the $b_n$ and $c_n$ data: this is useful if output is on disk or tape, to be used by program RCMBLN. The normal imput to the program consists of one card specifying input/output units, followed by one card containing the desired $n$ values, and then the entire deck of $b_n$ and $c_n$ values as provided. The Voigt function deck is inserted, if required, after the first 2 cards. The $b_n$ and $c_n$ data is in the form of blocks, each containing 61 cards. The order of the cards within each block must not be changed, but the blocks can be read in any order.

All the $b_n$ and $c_n$ values computed for case B are included as data with the simple run of the program described. The complete table of Voigt function values is provided with the sample run of program RCMBLN.

All information required for use of the program is given on comment cards, and a writeup is not required.

*Reference*

[1] M. Brocklehurst, Mon. Not. R. Astr. Soc. 148 (1970) 417.

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Computer Physics Communications 9 (1975) 268–269
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# ERRATUM NOTICE

*Title of manuscript*: A program to evaluate the reduced matrix elements of summations of one-particle tensor operators

*Author*: W.D. Robb

*Reference*: Computer Physics Communications 6 (1973) 132

*Title of program*: REDUCED TENSOR MATRIX ELEMENTS

*Catalogue number*: AAKF

Computer Physics Communications 9 (1975) 283–296
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# A PROGRAM PACKAGE FOR THE DIRICHLET PROBLEM WITH AXIALLY SYMMETRIC BOUNDARY CONDITIONS

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Received 25 October 1974

## PROGRAM SUMMARY

*Title of program*: DIRPAK

*Catalogue number*: ABSB

*Computer*: IBM 360/67; *Installation*: Computation Centre, National Research Council.

*Operating system*: TSS/360

*Programming language used*: FORTRAN IV

*High speed storage required*: 35000 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: 3

*Other peripherals used*: Card reader, line printer, disks in lieu of tapes

*No. of cards in combined program and test deck*: 2563

*Keywords*: Electrostatics, Laplace, Dirichlet problem, capacitance, axisymmetric, finite difference

*Nature of the physical problem*
In this communication, we describe accurate finite difference techniques for the solution of the Dirichlet problem in cylindrical coordinates with axially symmetric boundary conditions. The program package can be used for the calculation of the capacitance of ring capacitors.

*Method of solution*
Laplace's equation in cylindrical coordinates is replaced by a nine-point, finite difference approximation. At mesh points close to the boundary of the region, a nine-point, irregular difference approximation is used. The package allows for solution of the difference equations by successive overrelaxation (SOR) or by symmetric successive overrelaxation with semi-iterative refinement (SSOR-SI). The gradient of the potential is also approximated by nine-point differences. The total charge on a surface is obtained by integration, using Simpson's quadrature rule.

*Restrictions on the complexity of the problem*
The region where the Dirichlet problem is being solved cannot contain the axis of symmetry. The capacitor can consist of no more than six rings.

*Typical running time*
A boundary value problem was solved in an irregular region with 204 mesh points. The difference equations were solved by SOR iteration with a relaxation factor $\omega = 1.7$. The maximum residual of the difference equations was reduced to $10^{-8}$. The computing time for this example was approximately 12 seconds and the solution was accurate to 6 digits.

Computer Physics Communications 9 (1975) 297–304
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# RAPIDITY GENERATOR FOR MONTE-CARLO CALCULATIONS OF CYLINDRICAL PHASE SPACE

S. JADACH
*Institute of Physics, Jagellonian University, Cracow, Poland*

Received 1 November 1974

## PROGRAM SUMMARY

*Title of program*: GENRAP

*Catalogue number*: AAUO

*Computer*: CDC 7600; *Installation*: CERN, Geneva, Switzerland

*Operating system*: SCOPE 2.0

*Programming language used*: ANSI FORTRAN

*High speed storage required*: 6000 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 300

*Keywords*: Nuclear, high energy, hadrons, phase-space, Monte-Carlo, rapidity, integration, importance sampling.

*Nature of physical problem*
Analysis of high energy collisions of hadrons in the framework of many theoretical models needs numerical evaluation of multi-dimensional integrals over Lorentz invariant phase space. In practice, the only method of evaluating them exactly is the Monte-Carlo method. However, if we use methods of random generation of points in the phase space known up to now, the time of evaluation of these integrals increases not only with the number of particles, but also very rapidly with energy and Monte-Carlo calculations of phase space integrals for laboratory momentum over a thousand GeV/c are practically impossible.

*Method of solution*
The time of Monte-Carlo evaluation of integrals can be shortened by the importance sampling method [1]. The first step in solving the problem of importance sampling for calculation of the Lorentz invariant, cylindrical phase space was done by proposing the method of generation of the transverse momenta in a limited region [2]. However, even when this method is applied, the calculation time increases appreciably with increasing energy.

We present here a new method of solving this problem [3]. We propose to generate rapidity variable instead of longitudinal momenta [4], or some kind of intermediate masses [5]. When this method is applied the calculation time for a fixed number of outgoing particles remains nearly constant when the energy increases.

*Restriction on the complexity of the problem*
This program has a very good importance sampling for purely cylindrical phase space, i.e. for phase space with transverse momentum cut-off only. Deviations of the model from purely cylindrical phase space may decrease the efficiency of the program. The efficiency also decreases with increasing number of particles.

*Typical running time*
The generation time of one event is approximately proportional to the number of particles. However, at low energies there is a number of zero-weight events. The time of generation of one zero-weight event is shorter than that of non-zero-weight event. For example, the generation time of one event for 10 particles, for CDC 7600 computer at CERN is $2.3 \times 10^{-4}$ sec, and is nearly the same as in the case of a typical phase space Monte-Carlo program like FOWL [6];

*References*

[1] G.I. Kopylov, Osnovy kinematiki rezonansov, Moscow 1970.
[2] L. Van Hove, Nucl. Phys. B9 (1969) 331.
[3] S. Jadach, TPJU-10/73, July 1973, unpublished report.
[4] W. Kittel, W. Wójcik and L. Van Hove, Computer Phys. Commun. 1 (1970) 425.
[5] O. Pene and A. Krzywicki, Nucl. Phys. B12 (1969) 415.
[6] F. James, FOWL, A general Monte-Carlo phase space program, CERN Program Library W505.

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Computer Physics Communications 9 (1975) 305–311
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# COLOUR COORDINATE CALCULATIONS

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Received 14 October 1974

## PROGRAM SUMMARY

*Title of program*: COLOUR COORDINATE CALCULATIONS

*Catalogue number*: ACWA

*Computer*: ICL 1904A; *Installation*: Loughborough University of Technology

*Operating system*: GEORGE 2L

*Programming language used*: FORTRAN

*High speed storage required*: 5632

*No. of bits in a word*: 24

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader and line printer

*No. of cards in combined program and test deck*: 383

*Keywords*: Optics, colour, chromaticity coordinates, purity, dominant wavelength, trichromatic equation, chromaticity diagram, spectrum locus, C.I.E. Standard Observer, $(X, Y, Z)$ system.

*Nature of physical problem*
The two subroutines CHROME and CRODAT described in this paper can be used in conjunction to perform two tasks which arise in colorimetry. The first is to calculate the colour of a light source from its given spectral energy distribution. The second is to calculate the dominant wavelength and purity of a colour from its chromaticity coordinates.

*Method of solution*
The integrals giving the tristimulus values are evaluated by the trapezoidal rule using 5 nm steps, the distribution coefficients for the equal energy stimulus being taken as those for the C.I.E. standard observer (1931). The $(x, y, z)$ chromaticity coordinates are evaluated by normalising the tristimulus values and the dominant wavelength and purity calculated by transforming from a cartesian to a polar representation.

*Restrictions on the complexity of the problem*
The spectral energy distribution must be entered as an array of size (80), giving the energy at 5 nm intervals from 380 to 775 nm inclusive: no other range or interval is acceptable. This has been found to be satisfactory because the errors produced in the machine calculations are acceptable when compared with those arising in the practical measurement of colour. The program incorporates only the 1931 CIE Standard Observer data (for a 2° field) but this could easily be replaced by the 1964 CIE Supplementary Standard Observer data (for a 10° field) if required by the user.

*Typical running time*
Each call to the subroutine CHROME takes about $\frac{1}{2}$ sec on the ICL 1904A.

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Computer Physics Communications 9 (1975) 312–326
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# SYMMETRIZATION AND CALCULATION OF LEED INTENSITY PATTERNS

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Received 20 September 1974

## PROGRAM SUMMARY

*Title of program*: LEED BEAM-SYMMETRIZED

*Catalogue number*: ACKG

*Computer*: IBM 360/75; *Installation*: Royal Institute of Technology, Stockholm

*Operating system*: OS MVT

*Programming language used*: FORTRAN

*High speed storage required*: 194 kwords

*No. of bits in a word*: 32

*Overlay structure*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1989

*Reference to other published version of this program*: *Cat. no.*: ACKE; *Title*: LEED BY LAYERS AND PERTURBATION; *Ref. in CPC*: 7 (1974) 369.

*Keywords*: Solid state, surface structure, adsorbed layers, crystal symmetry, two-dimensional space groups, low energy electron diffraction, LEED, layer-by-layer method.

*Nature of the physical problem*
Experiments with low energy electron diffraction (LEED) are used for finding the composition of the unit mesh of crystal-overlayer (crystal *plus* overlayer) structures. For open structures having a large unit mesh the number of spots of the diffraction pattern rises rapidly with increasing energy. By performing the diffraction experiment at normal incidence the symmetry in the spot pattern can be utilized to reduce the number of beams to be calculated.

*Method of solution*
It is supposed that the crystal-overlayer structure can be sliced into well separated layers. The interaction of the beams of electrons with a particular layer is governed by von Laue's diffraction conditions characteristic of that layer [1]. The behaviour of von Laue's diffraction conditions under the operations of the two-dimensional space group of the crystal-overlayer structure is established by a group-theoretical method [2]. The method applies to dense or open crystal-overlayer structures having any of the 17 two-dimensional space group symmetries.

The LEED program [1] is extended to use the least possible number of beams for the calculation of symmetric intensity patterns. The program can be run both in a symmetrized and in an unsymmetrized mode.

*Restrictions on the complexity of the problem*
One atom per unit mesh of the individual layers; the unit mesh of the crystal-overlayer structure equal to that of the overlayer; 36 beams; 8 phase shifts.

*Typical running time*
Eg. for a primitive 2 × 2 structure on the (100) surface of a fcc crystal symmetrization will reduce 69 spots to 13 spots whose intensities are calculated in roughly 10 seconds on an IBM 360/75 computer, if 6 phase shifts are used. Parts of the program take times scaling as $(l+1)^4 p$ and $(l+1)^2 n^2 p$, where $l$ is the number of phase shifts minus unity, $n$ the number of beams or symmetrized combinations of beams and $p$ the crystal period normal to the surface.

*References*
[1] J. Rundgren and A. Salwén, Computer Phys. Commun. 7 (1974) 369.
[2] J. Rundgren and A. Salwén, J. Phys. C: Solid State Phys. 7 (1974) 4247.

Computer Physics Communications 9 (1975) 327–336
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# CONTINUUM EXCHANGE INTEGRALS FOR ALGEBRAIC VARIATIONAL CALCULATIONS OF ELECTRON–ATOM SCATTERING USING SLATER-TYPE ORBITALS AS BASIS FUNCTIONS*

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Received 8 January 1975

## ADAPTATION SUMMARY

*Title of adaptation:* NETI/ETI

*Adaptation number:* 0001

*Reference to original program:*
*Catalogue number:* AAGP; *Title:* NETI; *Ref. in CPC:* 5 (1973) 80; erratum; 8 (1974) 333.

*Authors of original program:* Richard L. Smith and Donald G. Truhlar

*Computer:* CDC CYBER 74; *Installation:* University Computer Center of the University of Minnesota

*Operating system:* KRONOS 2.1

*Programming language used:* FØRTRAN IV

*No. of bits in a word:* 60

*High speed storage required:* 14336

*Overlay structure:* None

*No. of magnetic tapes required:* None

*What other peripherals are used:* Card reader, line printer

*No. of cards required to effect adaptation (including directive cards):* 1120

*Keywords:* Atomic, exchange integrals, continuum wavefunctions, electron–atom scattering, variational method, spherical Bessel function, summation of series, numerical quadrature, recurrence relations, scattering amplitude.

*Nature of the physical problem*
The problem of electron scattering from atoms can be solved using algebraic variational methods [1,2]. The program NETI [3] computes the non-exchange integrals and the present adaptation NETI/ETI adds the facility to compute the two-electron free–free exchange integrals which are needed for algebraic variational scattering calculations including exchange when exponential-type functions and regular spherical Bessel functions are used as basis functions. The adapted program can be used to evaluate all the integrals needed for electron-atom scattering calculations by the standard algebraic variational methods using exponential-type functions and regular spherical Bessel functions as basis functions.

*Method of solution*
The exchange integrals are evaluated using the procedures of Lyons and Nesbet [4,5] with an improvement discussed in this article. In each case the subprogram XLN considers six available methods of computation and chooses the optimum one for the integral. The adaptation NETI/ETI uses subprograms of the previously published NETI [3] package for parts of the calculations of the exchange integrals.

*Restrictions on the complexity of the problem*
In the notation of Lyons and Nesbet [5], the program is restricted to non-negative integer values of $\lambda$, $\mu$, $p$, and $q$ while $k_1$, $k_2$, $\alpha$, and $\beta$ must be real and positive.

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* Research supported in part by the National Science Foundation under Research grant no. GP-28684.

*References*

[1] F.E. Harris and H.H. Michels, Methods Comp. Phys. 10 (1971) 144.
[2] D.G. Truhlar, J. Abdallah, Jr. and R.L. Smith, Advances in Chemical Physics 25 (1974) 211;
J. Abdallah, Jr. and D.G. Truhlar, J. Chem. Phys. 60 (1974) 4670.
[3] R.L. Smith and D.G. Truhlar, Computer Phys. Commun. 5 (1973) 80; erratum: 8 (1974) 333.
[4] J.D. Lyons and R.K. Nesbet, J. Comp. Phys. 4 (1969) 499.
[5] J.D. Lyons and R.K. Nesbet, J. Comp. Phys. 11 (1973) 166.

Computer Physics Communications 9 (1975) 351–359
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# A FORTRAN CODE FOR AUTOMATIC SPECTRUM ANALYSIS ON MEDIUM-SCALE COMPUTERS

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Received 25 January 1975

## PROGRAM SUMMARY

*Title of program*: PEAK2

*Catalogue number*: ABML

*Computer*: IBM 370/155 and 370/158; *Installation*: The University of Akron, Akron, Ohio, USA

*Operating system*: OS/MVT

*Programming language used*: FORTRAN IV (G)

*High-speed store required*: 14,000 words (56 kbt) at execution time

*Number of bits in a word*: 32

*Overlay structure*: None

*Number of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*Number of cards in combined program and test deck*: 1290

*Keywords*: Nuclear, automatic peak detection, additive convolution, doublet resolution, lorentzian fit, gaussian fit, spectroscopy, gamma ray, neutron activation, infrared, nuclear resonance, Mössbauer, particle size.

*Nature of physical problem*
The program performs fully automatic detection, description, and fitting of peaks (including doublets) in digital $X-Y$ spectra of various kinds, given only an approximate width, and the choice of positive or negative (absorption) height, of the peaks.

*Method of solution*
Peak detection is performed by additive convolution with a zero-area function [1]. The peak region just detected is conventionally described and its singlet or doublet nature decided. Gaussian or lorentzian peak region fit after background subtraction is performed [2]; in the doublet case the fit is iterative. Spectral smoothing before, and plotting after, processing are vailable; spectra are processed automatically in a single pass. The emphasis on economic use of memory is retained [1,2].

*Restrictions on program complexity*
The dimensions, such as 1024 spectral points, and 100 peak regions (for plotting purposes only), are easily changed together with some preliminary checks.

*Typical running time*
On an IBM 370/158 compilation (G) takes 18 CPU seconds. A 1024 channel spectrum with 30 peaks, including 18 doublets (fwhm $\simeq$ 4 channels) is processed in 11 CPU seconds. A 256-channel Mössbauer 6-line calibration spectrum uses 4 CPU seconds (see also sec. 5).

*Unusual features of the program*
Based on the methods described in refs. [1,2], the program is intended to be used either as it is, or as a basis for adaptation of its methods to spectral analysis on smaller computers and/or in real time. The main attributes of the minicomputer code [1,2] have been retained with many refinements. New features include a (non-essential) plotting facility, regional linear variability of the expected peak fwhm, optional spectral ($X$) compression to reduce processing time, linear channel calibration ($X_i = a + ib$), and choices of positive or negative peak height, gaussian or lorentzian peak shape, and regionally constant $Y$-uncertainty or counting statistics.

*References*

[1] E. von Meerwall and M.D. Gawlik, Computer Phys. Commun. 5 (1973) 309.
[2] E. von Meerwall and M.D. Gawlik, Computer Phys. Commun. 7 (1974) 115; also Bull. Am. Phys. Soc. II 19 (1974) 174.

Computer Physics Communications 9 (1975) 360–369
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# A GENERAL PURPOSE MONTE-CARLO PROGRAM

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Received 28 November 1974

## PROGRAM SUMMARY

*Title of program*: ERRCAL

*Catalogue number*: AAUP

| *Computer*: | *Installation*: |
|---|---|
| CDC 6600 | Data Center CDC, Rijswijk, The Netherlands |
| Burroughs B 6700 | Mons University Computing Center |

*Operating system*: SCOPE for CDC. MCP for Burroughs

*Programming language*: FORTRAN IV

*High speed store required*: 15000 words (CDC 6600)

*No. of bits in a word*: 60 (CDC 6600)

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 699

*Keywords*: Nuclear, high energy, statistics, simulation, Monte-Carlo, random.

*Nature of the physical problem*
This program is designed to estimate the propagation of errors and to simulate simple stochastic processes.

*Method of solution*
The program generates the distribution associated with a function of several random variables which is coded by the user. The distributions followed by the random variables are specified either by an analytical formula or numerically. The variables are generated by a Monte-Carlo method.

*Restrictions on the complexity of the problem*
The random variables must be uncorrelated.

*Typical running time*
The high-energy physics problem given as the second test run takes about 5.6 sec CP time on CDC 6600 for 5000 events generated. In fact, the running time depends primarily on the number of random variables and the complexity of the function coded by the user.

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# A NEW VERSION OF AAKF (Reduced Tensor Matrix Elements) ADAPTED TO SPECTROSCOPIC NOTATION

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Received 17 July 1974
Revised manuscript received 6 May 1975

## PROGRAM SUMMARY

*Title of program*: REDUCED TENSOR MATRIX ELEMENTS 2

*Catalogue number*: AAKP

| *Computer*: | *Installation*: |
|---|---|
| IBM 360/75 | University of Waterloo, Waterloo, Ont. Canada |

*Operating system*: 0S/360 HASP II

*Programming languages used*: FORTRAN IV

*High speed store required*: 102 K bytes

*No. of bits per byte*: 8

*Overlay structure*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1524

*CPC Library subprograms used*:

| *Cat. numbers* | *Titles* | *Refs. in C.P.C.* |
|---|---|---|
| ACQB | P SHELL CFP | 1 (1969) 15 |
| ACRN | A NEW D SHELL CFP | 6 (1973) 88 |
| AAGD | NJSYM | 1 (1970) 241,<br>2 (1971) 173 |
| AAGD0001 | ADAPT NJSYM FOR WEIGHTS | 2 (1971) 180 |
| AAGD0002 | ADAPT TO INTEGER ARITHMETIC | 5 (1973) 161 |

*Reference to other published version of this program: Catalogue number*: AAKF; *Title*: REDUCED TENSOR MATRIX ELEMENTS; *Ref. in C.P.C.*: 6 (1973) 132.

*Keywords*: Atomic, nuclear, transitions, electric multipole, magnetic multipole.

*Nature of the physical problem*
This program is a revision of Robb's [1] TENSOR program which enables one to calculate reduced matrix elements of sum-mations of one-particle tensor operators: recent corrections [2] are included.

*Purpose of the revision*
The purpose of the revision is two fold. Firstly, the formats for the input data and the printed output are changed to more compact and readable spectroscopic notation. Secondly, it modifies the punched output format so that the results may be read directly by other programs such as a transition probability program [3].

*Typical running time*
For the test data provided the program required 0.94 seconds to complete the calculations on IBM S360/75, Hasp. II.

*References*
[1] W.D. Robb, Computer Phys. Commun. 6 (1973) 132.
[2] W.D. Robb, Computer Phys. Commun. 9 (1975) 268.
[3] C. Froese Fischer and K.M.S. Saxena, Computer Phys. Commun. 9 (1975) 381.

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Computer Physics Communications 9 (1975) 381–391
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# OSCILLATOR STRENGTHS FROM NUMERICAL MCHF RADIAL FUNCTIONS

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Received 29 October 1974
Revised manuscript received 5 March 1975

## PROGRAM SUMMARY

*Title of program*: GF VALUES

*Catalogue number*: ACRZ

*Computer*: IBM S360/75; *Installation*: University of Waterloo, Waterloo, Ontario, Canada

*Operating system*: Hasp II

*Programming language used*: FORTRAN IV

*High speed core required*: 134 K bytes

*Number of bits in a byte*: 8

*Overlay structure*: None

*Number of magnetic tapes required*: None

*Other peripherals required*: Card reader, printer; disk (optional)

*Number of cards in the combined program and test deck*: 903

*CPC Library subprograms used (to supply data)*

| *Cat. numbers* | *Titles* | *Refs. in C.P.C.* |
|---|---|---|
| ACRF | MCHF 72 | 4 (1972) 107,<br>7 (1974) 236 |
| AAKP | REDUCED TENSOR MATRIX ELEMENTS 2 | 9 (1975) 370 |

*Keywords*: Atomic, oscillator strengths, *gf* values, length and velocity forms, atomic transitions

*Nature of physical problem*
The program computes *gf* values for transitions using results from MCHF72 [1] to define the initial and final states. A modified version of Robb's TENSOR program [2,3] provides some additional input data for the calculation. Both length and velocity forms are computed.

*Method of solution*
Since the radial functions are given in tabular form, all integrals are evaluated numerically. Simpson's rule is used for the transition integral of the length form, but a special formula was derived for the velocity form, so that the numerical procedure would preserve the symmetry property of the integral.

*Restrictions on the complexity of the problem*
The dimensions of the program allow up to 50 radial functions in the initial and/or final state combined, and up to 30 configurations in each of the initial and final states. These can readily be changed.

*Typical running time*
The CPU time required for the two sets of calculations mentioned in the test run was 1.8 seconds on the IBM System 360/75.

*References*

[1] C. Froese Fischer, Computer Phys. Commun. 4 (1972) 107; 7 (1974) 236.
[2] W.D. Robb, Computer Phys. Commun. 6 (1973) 132; 9 (1975) 268.
[3] C. Froese Fischer and K.M.S. Saxena, Computer Phys. Commun. 9 (1975) 370.

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Computer Physics Communications 9 (1975) 392–407
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# A COMPUTER PROGRAM FOR INTERNAL CONVERSION COEFFICIENTS AND PARTICLE PARAMETERS

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and

U. RAFF
*Institut für Physik der Universität Basel, Theoretische Physik, Klingelbergstr. 82, CH-4056 Basel, Switzerland*

Received 24 March 1975

## PROGRAM SUMMARY

*Title of program*: CATAR

*Catalogue number*: ABGP

*Computer*: UNIVAC 1108; *Installation*: Sandoz A.G., Basel, Switzerland

*Operating system*: EXEC 8

*Programming language used*: FORTRAN IV

*High speed store required*: 26K words

*No. of bits in a word*: 36

*Overlay structure*: None

*Number of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*Number of cards in combined program and test deck*: 3136

*Keywords*: Nuclear, atomic, Dirac equation, atomic shells, screening, internal conversion coefficient, electric multipoles, magnetic multipole transitions, internal conversion particle parameters, penetration effects.

*Nature of the physical problem*
CATAR calculates internal conversion coefficients and particle parameters for electric and magnetic multipole transitions. The dynamic effects describing the interaction of the shell electrons with the nuclear charge and currents give rise to additional transition matrix elements (penetration matrix elements) through which the internal conversion process depends on the structure of the nucleus. The electric monopole (E0) internal conversion transition that is the most important penetration effect is also taken into account.

*Method of solution*
The Dirac equation is solved numerically for the bound and the free electron states in a central field with a Hartree–Fock–Slater screening function given by input. The radial matrix elements for electric and magnetic multipole transitions are calculated simultaneously for all multipole orders and partial waves allowed by selection rules for each transition energy and atomic subshell.

*Restrictions on the complexity of the problem*
The program should work for all nuclear charge numbers $Z$ between $2 \leqslant Z \leqslant 126$ and all atomic shells. The number of highest multipole order is restricted to $L = 6$. The energy of the electron should be larger than 50 eV and less than 5 MeV. The gamma transition $k_\gamma$ must be within these limits, correspondingly. The function describing the screening of the nuclear charge by the atomic electrons ("screening function") must be given by input. For convenience the program has an option for a built-in, but approximate screening function, i.e., the analytical expression of Gaspàr [1].

*Reference*

[1] H.C. Pauli, K. Alder and R.M. Steffen, in: The electromagnetic interactions in nuclear physics, ed. W.D. Hamilton (North-Holland, Amsterdam, 1975) ch. 10.

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Computer Physics Communications 10 (1975) 1–10
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# EIGENSTATES AND EIGENVALUES OF LABELLING OPERATORS FOR O(3) BASES OF U(3) REPRESENTATIONS *

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Received 11 March 1975

## PROGRAM SUMMARY

*Title of program*: EIGLAB

*Catalogue number*: ABID

*Computer*: CDC Cyber 74. *Installation*: Centre de Calcul, Université de Montréal, Montréal, Québec, Canada.

*Operating system*: Scope 3.4.

*Programming language used*: FORTRAN

*High speed storage required*: 114000 words.

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1160

*Keywords*: Nuclear, high energy, atomic, representation, $U(3)$, $O(3)$, Lie group, eigenvalues, eigenstates, labelling operator, Lie algebra.

*Nature of the physical problem*
Basis states of $U(3)$ in the $O(3)$ representation are required to describe certain atomic nuclear or multipion states; $U(3)$ can refer to dynamical or permutation symmetries, $O(3)$ to angular momentum or isospin. EIGLAB computes such states as eigenstates of an $O(3)$ scalar labelling operator $Q$ in the enveloping algebra of $U(3)$.

*Method of solution*
The program calculates the matrices for $L^{(2)}$ and the labelling operator $Q$ in the Gel'fand basis of an arbitrary $U(3)$ representation and computes their eigenvalues and common eigenstates.

*Restrictions on the complexity of the problem*
(i) The labelling operator $Q$ must have the form

$$AX^{(3)} + BX^{(4)} + \tfrac{1}{2}C(X^{(3)}X^{(4)} + X^{(4)}X^{(3)}) + D(X^{(3)})^2 + E(X^{(4)})^2 + FL^{(2)}$$

(ii) The number of irreducible $O(3)$ representations in the $U(3)$ representation is $\leqslant 50$.

*Typical running time*
Compile time was 6.7 sec, total execution time for the test runs was 26.1 sec. Execution time for table 2 with $Q$ = LTL for the representation (18, 9, 0) was 45 sec.

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* Supported by the National Research Council of Canada and the "Ministère de l'Education du Québec".

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Computer Physics Communications 10 (1975) 11–29
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# THALIA – A ONE-DIMENSIONAL MAGNETOHYDRODYNAMIC STABILITY PROGRAM USING THE METHOD OF FINITE ELEMENTS

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and

K.V. ROBERTS
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Received 10 March 1975

## PROGRAM SUMMARY

*Title of program*: THALIA

*Catalogue number*: ACWB

*Computer*: CDC Cyber 7326; *Installation*: Ecole Polytechnique Fédérale, Lausanne

*Operating system*: SCOPE 3.4.2

*Programming language used*: FORTRAN

*High speed store required*: 25088 words (loader included)

*No. of bits in a word*: 60

*No. of magnetic tapes required*: None

*Other peripherals used*: Line printer, 1 disk file

*No. of cards in combined program and test deck*: 2636

*CPC Library subprogram used*:

| *Cat. number* | *Title* | *Refs. in CDC* |
|---|---|---|
| ABUK | OLYMPUS FOR CDC 6500 | To be published. |
| ACWC | HYMNIA | 10 (1975) 30. |

*Keywords*: Plasma physics, ideal MHD, variational principle, finite elements, spectrum, instabilities, eigenfunctions

*Nature of the physical problem*
The lifetime of a magnetically-confined plasma column depends critically on the growth rates of any unstable eigenmodes. The plasma is considered here as a one-component fluid described by the ideal one-dimensional MHD equations [1]. Purely oscillating or purely growing and damped modes can be studied by linearising these equations and perturbing an equilibrium state of the column. Not only the purely growing modes, i.e. the unstable eigenfunctions, but also stable, purely oscillating modes can be of interest [2]. THALIA has been written to find the whole spectrum from the variational principle [3].

*Method of solution*
The linearized ideal one-dimensional MHD equations are treated in variational form [3] by the method of finite elements [4]. In order to describe certain features of the problem with sufficient accuracy (for example: a displacement vector which satisfies div $\boldsymbol{\xi} \simeq 0$ for the fixed boundary case), we perform a rather general transformation and choose our basis functions from a class able to represent div $\boldsymbol{\xi} = 0$ everywhere. The eigenvalue problem $Ax = \omega^2 Bx$ is solved by SIVI, a subprogram of the band matrix library HYMNIA [5].

*Typical running time*
The time required is proportional to the number of intervals, to the number of wanted eigenvalues and to the number of iterations. A typical case with 100 intervals, 20 iteration steps takes about 10 seconds per eigenvalue.

*Unusual features of the program*
THALIA uses the CDC OLYMPUS package [6], and follows all prescriptions of the OLYMPUS system [7]. The code is written in STANDARD FORTRAN [8], except for the use of the input facility NAMELIST which is available on most computers, and is optimized for speed and memory requirements. Memory requirements are reduced by storing only half the band-width for the symmetric band matrices $A$ and $B$. For detecting a singular $A$ or a degenerate eigenvalue problem in SIVI a machine dependent parameter EPSMAC has to be defined. EPSMAC is set to be $10^{-12}$ for a CDC 6500.

*References*

[1] B.B. Kadomtsev, Reviews of Plasma Physics (Consultants Bureau, New York, 1966), Vol. 2, p. 155.

[2] W. Grossmann, M. Kaufmann and J. Neuhauser, Nucl. Fusion 13 (1973) 462.

[3] W.A. Newcomb, Ann. Physics 10 (1960) 232.

[4] G. Strang and G.J. Fix, An Analysis of the Finite Element Method (Prentice-Hall, Inc., Englewood Cliffs, New York, 1973).

[5] R. Gruber, Computer Phys. Commun. 10 (1975) 30.

[6] M.H. Hughes, Computer Phys. Commun. (to be published).

[7] K.V. Roberts, Computer Phys. Commun. 7 (1974) 237.

[8] Standard Fortran programming manual, Computer Standards Series, National Computing Centre Ltd., Manchester, England (1970).

Computer Physics Communications 10 (1975) 30–41
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# HYMNIA – BAND MATRIX PACKAGE FOR SOLVING EIGENVALUE PROBLEMS

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*Centre de Recherches en Physique des Plasmas, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

Received 10 March 1975

## PROGRAM SUMMARY

*Title of program*: HYMNIA

*Catalogue number*: ACWC

*Computer*: CDC Cyber 7326; *Installation*: Ecole Polytechnique Fédérale, Lausanne

*Operating system*: SCOPE 3.4.2

*Programming language used*: FORTRAN

*High speed store required*: 18944 words (Loader included)

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Line printer, 1 disk file

*No. of cards in combined program and test deck*: 2390

*CPC Library subprograms used*: None

*Keywords*: General purpose, numerical mathematics, eigenvalue problem, inverse iteration, band matrix, hermitian matrix.

*Nature of the physical problem*
Stability problems in physics or engineering such as those solved in [1–3] lead to eigenvalue problems of the type $Ax = \lambda Bx$, where $B$ is positive definite and $A$ can either be real symmetric or hermitian. Both matrices have a band structure.

*Method of solution*
HYMNIA is a band matrix package which solves the above-mentioned eigenvalue problem by the method of simultaneous inverse vector iteration [4]. Only the eigenvalues with lowest absolute value are obtained directly, but with an eigenvalue shift $\lambda_0$ it is possible to get any of them.

The advantage of HYMNIA, which is also the name of the CDC main program that tests the two main subprograms ⟨SIVI⟩ and ⟨CSIVI⟩,* is that all operations are performed within the half bandwidth $m$ of the one-dimensionally stored matrices $A$ and $B$ of order $n$. By decomposing the matrices ($\sim nm^2$ operations) before the iteration, only a number of point operations proportional to $nm$ has to be performed for the iteration part. The NEG facility gives the number of negative eigenvalues for the shifted problem and thus enables us to know which eigenvalue has been calculated.

⟨SIVI⟩ not only solves the eigenvalue problem, but can also be used simply to decompose $A$ and/or $B$. The cases of singular $A$ and non-positive $B$ are detected and diagnosed. Convergence information is given by the parameters NCONV and CONV.

*Restrictions on the complexity of the problem*
The matrix $B$ has to be real symmetric and positive definite. The matrix $A$ can either be real symmetric ⟨SIVI⟩ or hermitian ⟨CSIVI⟩. Both, $A$ and $B$ have to have a band structure.

*Unusual features of the program*
The test program HYMNIA reads input data using NAMELIST, which is not STANDARD FORTRAN but is available on most computers. Another non-standard utility is the CDC random generator RANF called by the subprograms ⟨SIVI⟩, ⟨CSIVI⟩, ⟨ORNOS⟩ and ⟨CORNOS⟩.

*References*
[1] T. Takeda, Y. Shimomura, M. Ohta and M. Yoshikawa, Phys. Fluids 15 (1972) 2193.
[2] K. Appert, D. Berger, R. Gruber and J. Rappaz, LRP 83/74 EPF-Lausanne, CRPP, submitted to J. Comp. Phys.
[3] K. Appert, D. Berger, R. Gruber, F. Troyon and K.V. Roberts, Computer Phys. Comm. 10 (1975) 11.
[4] J.H. Wilkinson, The Algebraic Eigenvalue Problem (Clarendon Press, Oxford, 1965).

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* References to subprogram names are in angular brackets ⟨ ⟩. Those with prefix "C" refer to the hermitian case and use complex arithmetic.

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# A PROGRAM FOR THE CALCULATION OF X-RAY REFLECTION INTENSITIES, Part 2

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Received 5 November 1974

## PROGRAM SUMMARY

*Title of program*: FIREFLY IV

*Catalogue number*: AAQC

*Computer*: ICL 4–72; *Installation*: UKAEA, Risley, UK

*Operating system*: 4J

*Programming language used*: FORTRAN IV

*High speed storage required*: 391 K bytes

*No. of bits in a byte*: 8

*Overlay structure*: None

*No. of magnetic tapes required*: 1

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 4551

*CPC Library subprograms used*:
*Catalogue number*: AAQB; *Title*: FIREFLY II; *Ref. in CPC*: 5 (1973) 328

*Reference to other published version of this program*:
*Catalogue number*: AAQB; *Title*: FIREFLY II; *Ref. in CPC*: 5 (1973) 328

*Keywords*: Crystallography, intensities, X-ray, powder diffraction, structure factor, crystal structure, dispersion correction.

*Nature of physical problem*
The program, FIREFLY IV, an extension of FIREFLY II, calculates the intensities of X-ray reflections with especial reference to the powder method. The program is very flexible and allows the intensity of reflections with given Miller indices to be calculated if the unit cell and its contents are specified together with the equipment used and, if necessary, temperature and absorption factors. Provision is made for the comparison of observed and calculated data. The most significant differences from FIREFLY II are that FIREFLY IV can: automatically centre the atoms in the unit cell, deal with fractional coordinates and, most important, apply a dispersion correction to the calculated intensities.

*Method of solution*
The Bragg reflection intensities are calculated by the standard formulae of X-ray diffraction as applied to X-ray powder diffraction.

*Restrictions on the complexity of the problem*
The program is written to manipulate up to 999 sets of Miller indices, 2000 atoms with coordinates $x_n$, $y_n$ and $z_n$, not greater than 100 atom types, 10 wavelengths and up to 9990 observed intensities and angles.

*Typical running time*
5 seconds for a typical example.

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# REDUCED MATRIX ELEMENTS OF SUMMATIONS OF ONE-PARTICLE TENSOR PRODUCTS

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Received 9 October 1974
Revised manuscript received 28 March 1975

## ADAPTATION SUMMARY

*Title of adaptation*: WKAPPAKQ

*Adaptation number*: 0001

*Reference to original program*: *Catalogue number*: AAKL;
*Title*: SPINORBITWEIGHTS;
*Ref. in CPC*: 9 (1975) 102.

*Authors of original program*: W.-D. Klotz

*High speed store required*: 2300 words

*No. of bits in a word*: 60

*Other peripherals used*: Card reader, line printer, card punch

*No. of cards required to effect adaptation (including directive cards)*: 263

*CPC Library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAGD | NJSYM | 1 (1970) 241,<br>2 (1971) 173 |
| ACQB | P SHELL C.F.P. | 1 (1969) 15 |
| ACQC * | D SHELL C.F.P. | 1 (1969) 16 |

*Additional keywords*: Atomic, one-body interaction, transition probabilities, multipoles, multipole radiation, hfs-interaction, effective operator approach, relativistic interactions

*Nature of the physical problem*
This adaptation is a generalization of the program SPINORBITWEIGHTS and calculates the reduced matrix elements of a general tensor operator $w^{(\kappa k)q}$, which may be written as a sum of $N$ one-particle tensor operators $w_i^{(\kappa k)q}$, as defined exactly by Armstrong and Feneuille [1]. The operator $w^{(\kappa k)q}$ is a "spin × orbital" tensor product with rank $\kappa$ in the spin space and rank $k$ in the orbital space. The matrix elements will be calculated to the same basis set of configuration wave functions as described in the early code. With the use of this program any one-particle interaction in an $N$-electron atom, like multipole radiation or hyperfine structure interactions, may be calculated in a very efficient way.

*Restrictions on the complexity of the problem*
The program is restricted to configurations with any number of s-, p- and d-electrons, but no more than two electrons in any shell of higher orbital angular momentum. The wave functions are restricted to pure $LS$-coupling.

*Typical running rime*
The execution time for the test run is 13.6 sec. During that time 165 matrix elements are calculated.

*References*

[1] L. Armstrong, Jr., Theory of Hyperfine Structure of free Atoms (Wiley-Interscience, 1971);
S. Feneuille, J. Phys. Radium 28 (1967) 61.

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[*] This program may be replaced by its new version ACRN [Computer Phys. Commun. 6 (1973) 88].

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# SYMMETRY AND BANDSTRUCTURE

J.Th.M. DE HOSSON
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Received 17 December 1974

## ADAPTATION SUMMARY

*Title of adaptation*: SYMMETRY AND BANDSTRUCTURE

*Adaptation number*: 0001

*Reference to original program*: *Catalogue number*: ACMJ; *Title*: SYMMETRIZED APW; *Ref. in CPC*: 4 (1972) 361

*Authors of original program*: V. Hoffstein, D.K. Ray and M. Belakhovsky

*Computer*: Control Data CYBER 74

*Operating system*: SCOPE 3.4.1. level 373

*Programming language used in adapted program*: FORTRAN

*High speed storage required*: 70742 words

*No. of bits in a word*: 60

*No. of cards required to effect adaptation*: 39

*Nature of physical problem*
The program ACMJ (1) calculates the energy bands and electronic structure of cubic lattices with no more than two different atoms per unit cell.

*Method of solution*
The program was designed to run on an IBM computer and this adaptation converts it for use on CDC computers. The changes are also suitable for the program ACME [2].

The method of calculation of the bandstructure is the Symmetry Augmented Plane-Wave method (SAPW) which makes use of the point group symmetry of the hamiltonian.

*Restrictions on the complexity of the problem*
Only for cubic lattices.

*Typical running time*
For a 3 × 3 matrix eigenvalue problem calculated with ACMJ: 17 seconds with the FTN-compiler and 12 seconds with the RUN-compiler.

*References*

[1] V. Hoffstein, D.K. Ray, M. Belakhosvky, Computer Phys. Commun. 4 (1972) 361.
[2] V. Hoffstein and O. Moller, Computer Phys. Commun. 2 (1971) 17.

## ERRATUM NOTICE

*Title of manuscript*: A general program to calculate the matrix of the spin–orbit interaction

*Authors*: W.-D. Klotz

*Reference*: Computer Physics Communications 9 (1975) 102.

*Title of program*: SPINORBITWEIGHTS

*Catalogue number*: AAKL

*Title of manuscript*: Program for spectra and cross-section calculations within the pre-equilibrium model of nuclear reactions

*Author*: E. Běták

*Reference*: Computer Phys. Commun. 9 (1975) 92.

*Title of program*: PREEQ

*Catalogue number*: ABGO

Computer Physics Communications 10 (1975) 87–97
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# CALCULATIONS OF HARMONIC OSCILLATOR BRACKETS*

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*Center for Nuclear Studies, University of Texas, Austin, Texas 78712, USA*

Received 1 May 1975

## PROGRAM SUMMARY

*Title of program*: OSCILLATOR BRACKET

*Catalogue number*: ABPE

*Computer*: CDC 6600; *Installation*: University of Texas Computer Center

*Operating system*: CDC Scope

*Programming languages used*: FORTRAN IV

*High speed store required*: 35300 words

*Number of bits in a word*: 60

*Overlay structure*: None

*Number of magnetic tapes required*: None

*Other peripherals used*: Card reader and line printer

*Number of cards in combined program and test deck*: 943

*Keywords*: Nuclear, nuclear spectra, nuclear structure, nuclear reaction, shell model, Talmi coefficient, Brody–Moshinsky bracket, angular momentum, harmonic oscillator.

*Nature of the physical problem*
The oscillator brackets [1,2] are used in various aspects of nuclear structure and reaction calculations [1,2]. Our program calculates these very rapidly.

*Method of solution*
The method is to use a closed form for an oscillator bracket as given by Baranger and Davies [1], and then to calculate simultaneously a large number of brackets that have different sets of principal quantum numbers for a given set of angular-momentum quantum numbers.

*Restrictions on the complexity of the problem*
Restrictions come about only through the size of the core storage assigned by the DIMENSION statements. The storage presently assigned will meet the needs of most present day nuclear physics calculations.

*Typical running time*
The running time of the program ranges roughly from 600 to 1000 brackets per second of CP time on the CDC 6600 computer at the computer center of the University of Texas.

*References*

[1] M. Baranger and K.T.R. Davies, Nucl. Phys. 79 (1966) 403.
[2] M. Moshinsky, Nucl. Phys. 13 (1959) 104.

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* Work supported in part by the U.S.E.R.D.A.

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# INVERSION OF ABEL'S INTEGRAL EQUATION BY A DIRECT METHOD

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Received 1 May 1975

## PROGRAM SUMMARY

*Title of program*: ABEL

*Catalogue number*: ABSC

*Computer*: IBM 360/75; *Installation*: West Virginia University

*Operating system*: HASP

*Program language used*: FORTRAN IV

*High speed store required*: 17028

*No. of bits in a word*: 16

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program test deck*: 174

*Keywords*: Plasma, spectroscopy, Abel integral equation, product integration, spline interpolation

*Nature of physical problem*
Determination of the radial distribution of the emission coefficient from the measured intensity distribution when the sourc is thin and axially symmetrical

*Method of solution*
Abel's integral equation is inverted by a direct procedure using product integration. A procedure using splines is used for interpolating the data, which need not be equally spaced, to the needed points and to interpolate the solution to the desired output points. The integration is stopped a few steps short of the center because of the singularity and the solution is extrapolated by the spline procedure.

*Restrictions on the complexity of the problem*
The dimensioning of internal arrays limits the number of data points and the number of steps in the integration to 300 points also no provision is made for smoothing data.

*Typical running time*
6 seconds for five sets of data (31 points each) and 60 steps in integration.

*References*

[1] C. Fleurier and J. Chapelle, Computer Phys. Commun. 7 (1974) 200–206.

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* Present address: Department of Chemical Engineering, Kansas State University, Manhattan, KS66502, USA.

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# NORMAL COORDINATE ANALYSIS OF CRYSTALS

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Received 7 March 1975

## PROGRAM SUMMARY

*Title of program*: NORMAL COORDINATE ANALYSIS

*Catalogue number*: ACKJ

*Computer*: CYBER 74; *Installation*: State University Groningen

*Operating system*: SCOPE 3.4.1., level 373

*Program language used*: FORTRAN 4.1.

*High speed store required*: 155k (octal)

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*Number of cards in combined program and test deck*: 1325

*Keywords*: Solid state, dynamical matrix, normal coordinate analysis, infrared spectra analysis, eigenvalue problem, threshold Jacobi method, Householder procedure.

*Nature of the physical problem*
A program has been written for solving the vibrational secular equation in cartesian coordinates [1] and for adjusting a set of force constants to give a fit of calculated and observed frequencies [2] which are measured by means of infrared transmission spectroscopy.

*Method of solution*
Two methods for calculating the eigenvalues and eigenvectors are included in the program deck. These methods are: the threshold serial Jacobi method [3] and the Householder procedure [4]. Although the latter is faster than the Jacobi method, the eigenvectors are more accurate in the case of the threshold serial Jacobi procedure.

*Restriction on the complexity of the problem*
The program is dimensioned for 20 atoms per unit cell. The number of degrees of freedom may be increased to 99, depending on the available storage capacity.

*Typical running time*
For the eigenvalue problem solved by threshold serial Jacobi method for $KNiF_3$ (without iteration procedure): 12.6 sec.

*Unusual features of the program*
Using the symmetry coordinates, it is possible to diagonalize the dynamical matrix in blocks. The symmetry coordinates can be calculated in some cases by the method and the program given by Warren and Worlton [5], using a reducible multiplier representation of the point group of the wavevector ($k = \mathbf{0}$). However, the input of the symmetry coordinates is not necessary for our program. Block-diagonalization of the dynamical matrix set up in cartesian coordinates is often not very useful for solving the eigenvalue problem.

*References*

[1] T. Shimanouchi, M. Tsuboi and T. Miyazawa, J. Chem. Phys. 35 (1961) 1597.
[2] T. Shimanouchi and I. Suzuki, J. Chem. Phys. 42 (1965) 296.
[3] J.H. Wilkinson, The Algebraic Eigenvalue Problem (Clarendon Press, Oxford, 1965) p. 277.
[4] A.S. Householder, J. Ass. Comp. Mach. 5 (1958) 205–243, 335–342.
[5] J.L. Warren and T.G. Worlton, Computer Phys. Commun. 8 (1974) 71–84.

Computer Physics Communications 10 (1975) 117–132
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# TLASER – A $CO_2$ LASER KINETICS CODE

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*Department of Computing, Royal Holloway College, Englefield Green, Surrey, UK*

and

Kenneth SMITH and R.M. THOMSON
*Centre for Computer Studies, The University, Leeds, UK*

Received 26 March 1975

## PROGRAM SUMMARY

*Title of program*: TLASER

*Catalogue number*: ACWD

| *Computer*: | *Installation*: |
|---|---|
| ICL 1906A | University of Leeds Computing Centre |
| CDC 6600 | University of London Computing Centre |
| KDF9 | NPL, Teddington |

*Operating system*: George 4, Scope 3.4, Egtran

*Programming language used*: FORTRAN

*High speed store required*: 13K

*No. of bits in a word*: 48

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in a combined program and test deck*: 1117

*Keywords*: Laser model, $CO_2$, dissociation, power output

*Nature of the physical problem*
TLASER is a program which predicts the output power pulse and gain from a model of an electrically excited $CO_2$ gas laser, including the effects of dissociation and a variable ambient gas temperature. The laser medium consists of $CO_2$, $N_2$, He, and CO, the latter being introduced intentionally, or by dissociation of $CO_2$.

*Method of solution*
The laser medium is described by 8 main dependent variables, $E, E_1, E_2, E_3, E_4, E_5, I_v, N_{100}$ which represent respectively the energy of the translational plus rotational motion of the gas, the energies of the three vibrational modes of $CO_2$, the energies of the vibrational modes of $N_2$ and CO, the radiation intensity within the laser cavity and $N_{100}P(J+1)$ is the number of $CO_2$ molecules per unit volume in the rotational level $J(J+1)$ of the lowest symmetric mode. The model consists of eight coupled ordinary differential equations, each describing the rate of change of one of the above variables with time. These equations are solved initially by the Runge–Kutta method and subsequently by a modified Hamming predictor corrector method.

*Restrictions on the complexity of the problem*
The model used is a spatially independent one. Only the dominant energy exchange processes have been included and there is no analysis of the plasma properties other than these energy exchange processes. The degree of dissociation of $CO_2$ is input as data.

Either an analytic shape is assumed for the electron beam describing the number of electrons per unit volume as a function of time or experimental values can be read in.

*Typical running time*
Execution time for a complete solution of the power output profile over 1 μsec takes typically 7 secs on a CDC-6600 and 7 minutes on a KDF9.

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# A GENERAL-PURPOSE ROUTINE FOR THE ANALYSIS OF SPECTROSCOPIC PEAK SHAPES

E. von MEERWALL
*The University of Akron, Department of Physics, Akron, Ohio 44325, USA*

Received 8 September 1975

## PROGRAM SUMMARY

*Title of program*: SPEC3

*Catalogue number*: ABMM

*Computer*: IBM 370/158; *Installation*: The University of Akron, Akron, Ohio, U.S.A.

*Operating system*: OS/MVT or OS/VS2

*Programming language used*: FORTRAN IV (G)

*High speed store required*: 18000 words (70 kbt)

*Number of bits in a word*: 32

*Overlay structure*: None

*Number of tapes required*: None

*Other peripherals used*: Card reader, line printer (Calcomp incremental plotter, optional)

*Number of cards in combined program and test deck*: 1004

*Keywords*: Nuclear, spectroscopy, peak description, simulation, X-ray, magnetic, resonance, quadrupole.

*Nature of the physical problem*
The program analyzes spectroscopic peak shapes parametrically (eleven parameters). A simulated spectrum may be juxtaposed, adjusted variously, and similarly analyzed. Plotting is provided.

*Method of solution*
The spectral parameters are calculated from their definitions, using interpolation when necessary. The synthesis may be composed of a background plus either lorentzians, gaussians, or user-defined peak shapes.

*Restrictions on program complexity*
Present dimensions provide a maximum of 200 data points and a synthesis composed of 200 points containing up to 16 components. These limits may be changed by redimensioning and making minor alterations.

*Typical running time*
On an IBM 370/158, compilation takes 13 CPU seconds. Spectra containing from 40 to 100 points, generating syntheses and both line printer and Calcomp plots, are processed in less than 4 CPU seconds.

*Unusual features of the program*
The program is intended to analyze spectroscopic peak regions, and to allow comparisons with proposed line shape models. To facilitate this,

1. the program reads spectral data ($x_i$, $y_i$), where $x_i$ may be unequally spaced, and may be scaled and offset to correspond to actual spectral abscissa values,
2. the spectral preprocessor may be instructed to integrate the (derivative) spectrum (e.g., wide-line NMR) and adjust the background and its slope or curvature, and
3. the synthesis may be composed of lorentzian or gaussian components, or else of shapes defined by the user. It may be left fixed or else adjusted (height scaling, abscissa shift, abscissa scaling) to correspond more closely to the spectrum.

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# RAMSES, A TWO-DIMENSIONAL, PIC TYPE, LASER PULSE PROPAGATION CODE

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and

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*University of California, Los Alamos Scientific Laboratory,*
*Los Alamos, New Mexico 87544, USA*

Received 23 June 1975

## PROGRAM SUMMARY

*Title of program*: RAMSES

*Catalogue number*: ABUL

| *Computer*: | *Installation*: |
|---|---|
| ICL 4/70 | UKAEA Culham Laboratory |
| IBM 370/168 | KFA Jülich, W. Germany |

*Operating system*: ICL Multijob

*Programming language*: FORTRAN

*High speed store required*: 199680 bytes

*No. of bits in a byte*: 8

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Line printer

*No. of cards in combined program and test deck*: 3798

*CPC Library subprograms used*: *Cat. No.*: ABUF; *Title*: OLYMPUS; *Ref. in CPC*: 7 (1974) 254.

*Keywords*: Plasma physics, laser propagation, photons, particle code, 2D, simulation, trajectories, refraction, pulse, laser target, focusing, defocusing, OLYMPUS, laser fusion, fusion reactor, optics.

*Nature of the physical problem*
The model used in RAMSES is intended to study the propagation of a laser pulse through a background gas or plasma [1]. The laser pulse is composed of macroscopic photons whose trajectories are calculated. Gradients in the refractive index, which may be computed self-consistently from photo-ionization of the plasma, change the direction of the photons and this can lead to focusing or defocusing of the pulse. Rotational symmetry is assumed for both the laser pulse and the background. Computations with the model may support laser-fusion reactor studies and laser-target studies as well as general work on the propagation of laser light.

*Method of solution*
A particle simulation model has been applied to the problem of calculating the trajectories of macroscopic photons. The photons carry variable amounts of energy in order to obtain arbitrary pulse shapes. The model evaluates the refractive index from the local electron density which may be supplied either explicitly or calculated self-consistently from local densities and ionization rates. The gradients of the refractive index determine the photon motion using a two-step predictor-corrector scheme. Analytic functions for ionization rates, pulse shape and neutral and electron density profiles are tabled in appropriate FUNCTION subprograms which may be amended as necessary.

*Restrictions*
Only initially parallel or focused laser pulses can be computed. The background density is assumed to be time-independent if ionization is involved, but if the electron density is supplied explicitly it may also be time-dependent.

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* On leave from: Rheinisch Westfälische Technische Hochschule, Institut für Reaktortechnik, 51 Aachen, Fed. Rep. Germany.

*Unusual features*

RAMSES is written in Standard Fortran [2] except for the use of the NAMELIST facility. The structure of the program is based on the OLYMPUS system [3] which facilitates a transfer to other computers. The graphical output package is excluded since it makes use of the Culham GHOST system which is not generally available. SI units are used throughout the code [4].

*References*

[1] D.B. Henderson, Los Alamos Scientific Laboratory Report LA-5086 MS (1972);
D.B. Henderson, Nuclear Engineering Design 30 (1974) 111.

[2] Standard Fortran Programming Manual, Computing Standards Series, National Computing Centre Ltd, Manchester, England (1970).

[3] J.P. Christiansen and K.V. Roberts, Computer Phys. Commun. 7 (1974) 245.

[4] C.H. Page and P. Vigoureux, SI The International System of Units, National Physical Laboratory, London (1973).

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Computer Physics Communications 10 (1975) 167–181
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# OLYMPUS CONTROL AND UTILITY PACKAGE FOR THE CDC 6500

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and

G.G. LISTER
*FOM-Instituut voor Plasmafysica (Associatie Euratom-FOM), Jutphaas, Netherlands*

Received 27 August 1975

## PROGRAM SUMMARY

*Title of program*: OLYMPUS FOR CDC 6500

*Catalogue number*: ABUK

*Computer*: CDC 6500; *Installation*: SARA (Stichting Academisch Rekencentrum Amsterdam, Netherlands)

*Operating system*: SCOPE 3.4.1

*Programming languages used*: STANDARD FORTRAN, CDC Extended Fortran, Compass

*High speed store required*: 12614 words for the MINOS test program

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Line printer, disc

*No. of cards in combined program and test deck*: 2170

*Reference to other published versions of this program*:

| *Catalogue number* | *Title* | *Ref. in CPC* |
|---|---|---|
| ABUF | OLYMPUS | 7 (1974) 245 |
| ABUJ | OLYMPUS FOR IBM 370/165 | 9 (1975) 51 |

*Nature of the problem*
A standard methodology called the OLYMPUS system [1] has been established for constructing, testing and operating Fortran programs which solve equations describing initial-value problems. This system provides a clear standard structure for programs of a similar kind, and enables them to be transferred without difficulty from one type of computer to another provided that they are written in Standard Fortran [2]. Each program runs under the supervision of a standard control and utility package. Versions of the OLYMPUS system have previously been published for the ICL 4/70 [3] and IBM 360/370 series [4] computers, and the present package is the corresponding version for the CDC 6500 and other computers in the CDC range which use the SCOPE 3.4 operating system [5].

*Method*
Refs. [1,3,4] should be consulted for a fuller description of the OLYMPUS system and how it is used. Components of the package are stored in source and binary form in a local system library and brought into use by appropriate control statements. In the CDC version, COMMON blocks are inserted into subprograms by means of the CDC UPDATE [6] facility using * CALL control statements, so that a separate preprocessor [4] is not required.

*Restrictions*
Before the OLYMPUS package is used, the CPC numbering in columns 73–80 of the NAMELIST data statements and end-of-record (EOR) statements should be removed.

*References*
[1] K.V. Roberts, Computer Phys. Commun. 7 (1974) 237.

[2] Standard Fortran Programming Manual, Computer Standards Series, National Computing Centre Ltd., Manchester, England (1970).

[3] J.P. Christiansen and K.V. Roberts, Computer Phys. Commun. 7 (1974) 245.

[4] M.H. Hughes, P. Roberts and K.V. Roberts, Computer Phys. Commun. 9 (1975) 51.

[5] Scope Reference Manual, Models 72, 73, 74 Version 3.4.1, 6000 Version 3.4.1. Control Data Corporation, Publ. No. 60307200, Rev. 5 (1973).

[6] UPDATE Reference Manual, Control Data Corporation, Publ. No. 60342500, Rev. D (1974).

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# SOLUTION OF BOUND STATE PROBLEMS IN NUCLEAR SHELL MODELS WITH MOMENTUM DEPENDENT POTENTIALS

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Received 4 June 1974, revised manuscript received 9 September 1975

## PROGRAM SUMMARY

*Title of program*: NUCLEAR POTENTIAL

*Catalogue number*: ACWK

*Computer*: IBM 360/50; *Installation*: Texas Tech

*Operating system*: OS 360

*Programming language used*: FORTRAN IV (G)

*High speed storage required*: 21,553 words

*No. of bits in a word*: 32

*Overlay structure*: None

*Other peripherals used*: Card Reader and Punch; Line printer

*No. of cards in combined program and test deck*: 1349

*Keywords*: Nuclear, energy levels, wave functions, Morse function, analytic solution, Schrödinger equation, nonlocal potential, momentum-dependent potential, shell model.

*Nature of physical problem*
Investigations of the structure of nuclei show that a nonlocal effect should be included in the nucleon–nucleus or nucleon–nucleon interaction [1]. A nonlocal potential can be understood as reflecting the correlations existing in nuclear matter, whereby the presence of a particle at position $\boldsymbol{r}$ influences the probability of finding another nucleon at a point $\boldsymbol{r}'$ in the neighborhood of $\boldsymbol{r}$ [2]. This in turn affects the energy of the particle at $\boldsymbol{r}'$. The nonlocal potential can be expressed as an effective energy-dependent potential. From the effective potential, the single-particle wave functions and eigenvalues are calculated.

*Method of solution*
The effective potential is approximated by a function for which the Schrödinger equation is analytically solvable [3]. The wave function and eigenvalue are then expressable in terms of the parameters of the analytically solvable function. The program finds the values of the parameters that give a "best" fit to the effective potential and then computes the corresponding eigenvalue.

*Restrictions on the complexity of the problem*
The parameters of the effective potential are chosen to be suitable for nuclei along the beta stable line and with $A > 10$.

*Typical running time (IBM 360/50)*
The running time (IBM 360/50) for one single-particle state can range from 1–15 minutes. The variation in running time strongly depends on the number of iterations required for convergences and the number of points considered in the matching procedure. A good initial energy estimate significantly reduces the number of iterations, so an energy formula has been provided which generates a reasonably accurate estimate. The running time for the example is 1.3 minutes (2.8 minutes including compilation).

*Unusual features of the program*
The input data is read under the NAMELIST option of FORTRAN IV (G). The variable DUMMY is used for the sole purpose of reading the card identification/sequence field in columns 77–80. Under normal running conditions, the data cards will not be sequenced and the variable DUMMY can be eliminated.

*References*

[1] Intern. Conf. on The Nucleon–Nucleon Interaction, Rev. Mod. Phys. 39 No. 3 (1967).
[2] M.A. Preston, Physics of the Nucleus (Addison-Wesley, Reading, Mass., 1963) p. 192.
[3] M.A.K. Lodhi, Phys. Rev. 182 (1968) 1061;
M.A.K. Lodhi and B.T. Waak, Phys. Rev. Lett. 29 (1972) 301.

Computer Physics Communications 10 (1975) 194–202
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# DETERMINATION OF SSOR–SI ITERATION PARAMETERS

J.B. CAMPBELL
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Received 21 April 1975

## PROGRAM SUMMARY

*Tital of program*: MUCALC

*Catalogue number*: ABUM

*Computer*: IBM 360/67; *Installation*: Computation Centre, National Research Council

*Operating system*: TSS/360

*Programming language used*: FORTRAN IV

*High speed storage required*: 26161 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: 2 (disks may be used instead)

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1126

*Keywords*: Electrostatics, plasma physics, fluid dynamics, Laplace, Dirichlet problem, eigenvalue, fixed membrane, finite difference.

*Nature of the physical problem*
In this communication, we describe an efficient method for the determination of iteration parameters for symmetric successive overrelaxation iteration with semi-iterative refinement as applied to the solution of the discrete laplacian. SSOR–SI is one of the iterative techniques used in ref. [1] for the solution of finite-difference equations and is described by Young [2, p. 471]. The program may also be used to calculate at least one eigenvalue of the fixed membrane problem.

*Method of solution*
The spectral radius of the Jacobi matrix associated with the difference equations is determined by the power method described by Faddeev and Faddeeva [3, ch. V]. This value can be used for a determination of SSOR iteration parameters [2, p. 464].

*Restrictions on the complexity of the problem*
The iteration parameters are determined only for a region where there are no irregular difference approximations and where a square mesh is used.

*Typical running time*
The first eigenvalue of the fixed membrane problem for an L-shaped region was calculated to 3 significant digits in 10 sec. When assembler language versions of two small subroutines of the program were used, the computing time was reduced to 5 sec. An accuracy of 3 digits in the first eigenvalue is sufficient for the determination of iteration parameters.

*Special features*
Integer arithmetic is used throughout the determination. Integer multiplication and division occur in the key parts of the program only when the multiplier or divisor is a power of 2.

*References*

[1] J.B. Campbell, A program package for the Dirichlet problem with axially symmetric boundary conditions, Computer Phys. Commun. 9 (1975) 283.
[2] D.M. Young, Iterative Solution of Large Linear Systems (Academic Press, New York, 1971).
[3] D.K. Faddeev and V.N. Faddeeva, Computational Methods of Linear Algebra (W.H. Freeman and Co., San Francisco and London, 1963).

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Computer Physics Communications 10 (1975) 223–233
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# MULTISTATE MOLECULAR TREATMENT OF ATOMIC COLLISIONS IN THE IMPACT PARAMETER APPROXIMATION. I – INTEGRATION OF COUPLED EQUATIONS AND CALCULATION OF TRANSITION AMPLITUDES FOR THE STRAIGHT LINE CASE

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and

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Received 16 July 1975

## PROGRAM SUMMARY

*Title of program*: PAMPA

*Catalogue number*: ACWJ

| *Computer*: | *Installation*: |
|---|---|
| IRIS 80 | Centre de Calcul Interuniversitaire, Bordeaux, France |
| IBM 360–65 | Observatoire de Paris, France |
| IBM 370–165 | CIRCE, Orsay, France |
| IBM 360–44 | Facultad de Medecina, Universidad Nacional de Buenos-Aires, Argentina |

*Operating system*: SIRIS 8, HASP

*Program language used*: FORTRAN

*High speed storage required*: 16K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 877

*Keywords*: Atomic, molecular, collisions, impact-parameter method, eikonal, semi-classical, coupled equations.

*Nature of the physical problem*
Multistate molecular treatment of atomic collisions in the impact parameter approximation. Calculation of the transition amplitudes for the straight-line case.

*Method of solution*
The coupled first-order differential equations are integrated by the method of Bulirsch and Stoer. The integrals over energy differences are integrated by Simpson's rule.

*Restriction on the complexity of the problem*
Linear trajectories only.

*Typical running time*
Running times for the test run: on the IRIS 80: 0.65 minutes, on the IBM 360–65: 48 seconds, on the IBM 370–165: 34 seconds.

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# CALCULATION OF CANTERBURY APPROXIMANTS

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*Mathematical Institute, University of Kent,*
*Canterbury, Kent, UK*

Received 18 June 1975

## PROGRAM SUMMARY

*Title of program*: FORTRAN CALCULATION OF C.A's

*Catalogue number*: ACWF

*Computer*: ICL 4130; *Installation*: University of Kent

*Operating system*: DES 2

*Programming language used*: FORTRAN IV

*High speed storage required*: 5000 words

*No. of bits in a word*: 24

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 410

*Reference to other published version of this program*: *Catalogue number*: ACWG; *Title*: ALGOL CALCULATION OF C.A's; *Ref. in CPC*: this paper.

*Keywords*: General purpose, rational, approximant, Chisholm, Hughes Jones, Padé, general off diagonal, prong, perturbation series.

## PROGRAM SUMMARY

*Title of program*: ALGOL CALCULATION OF C.A's

*Catalogue number*: ACWG

*Computer*: ICL 4130; *Installation*: University of Kent

*Operating system*: DES 2

*Programming language used*: ALGOL 60

*High speed storage required*: 7000 words

*No. of bits in a word*: 24

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 411

*Reference to other published version of this program*: *Catalogue number*: ACWF; *Title*: FORTRAN CALCULATION OF C.A's; *Ref. in CPC*: this paper

*Keywords*: General purpose, rational, approximant, Chisholm, Hughes Jones, Padé, general off diagonal, prong, pertubation series.

*Nature of physical problem*
These approximants may be applied for resummation of the perturbation series with two interaction hamiltonians, e.g. that in potential scattering given by the sum of an attractive and a repulsive Yukawa potential [1]. Many other applications are envisaged, especially in the field of critical phenomena [2], and fluid flow.

*Method of solution*
Prong methods [3].

*Restriction on the complexity of the problem*
The problem must be well-conditioned.

*Tyical running time*
$(NX+NY)^4\ 10^{-2}$ sec approximately.

*References*

[1] P.R. Graves–Morris and S. Samwell, Kent preprint (1975).

[2] D.W. Wood and H.P. Griffiths, J. Phys. A (Lett.) 7 (1974) L101;
D.E. Roberts, D.W. Wood and H.P. Griffiths, J. Phys. A 8 (1975) 1365.
P. Fox and D.W. Wood, submitted to J. Phys. A8 (1975) 1761.

[3] R. Hughes Jones and G.J. Makinson, J. Inst. Maths. Applics. 13 (1974) 299.

Computer Physics Communications 10 (1975) 245–250
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# EXPLICIT FORMULAS FOR CLEBSCH–GORDAN COEFFICIENTS

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Haifa, Israel*

Received 12 November 1974, revised manuscript received 17 July 1975

## PROGRAM SUMMARY

*Title of program*: CLEBSCH–GORDAN EXPLICIT FORMULAS

*Catalogue number*: ACWL

*Computer*: IBM 370/168: *Installation*: Technion Computer Center, Haifa, Israel

*Operating system*: OS-MVT-Rsl. 7 + HASP, Formac system (Minimac etc.), PL1/F compiler

*Program language used*: FORMAC (includes PL1)

*High speed storage required*: 65,536 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 170

*Keywords*: Atomic, nuclear, Clebsch–Gordan, spectroscopy, algebraic manipulation, Formac.

*Nature of the physical problem*
To obtain explicit algebraic formulas for Clebsch–Gordan coefficients for high values of angular momentum.

*Method of solution*
Algebraic method based on the Racah formula using the FORMAC programming language.

*Restriction on the complexity of the problem*
Formac limitations. Numbers which are too large may be generated during intermediate stages of the program for high values of angular momentum.

*Typical running time*
Compilation and linkage: 7 seconds

*Execution time*
Depending on the values demanded: 11 seconds for $j_2 = 1/2, 3/2$; 6 minutes for $j_2 = 2, 5/2, 3, 7/2, 4, 9/2$.

*Unusual features of the program*
The results are algebraic formulas in which numbers can be substituted to get numerical results.

*References*

[1] PL/I-FORMAC Symbolic Mathematic Interpreter IBM Corporation, Program Information Department (PID), 40 Saw Mill River Road, Hawthorne, New York 10532, USA.
[2] A. Messiah, Mécanique Quantique (Dunod, Paris, 1960) Appendix C.

## ERRATUM NOTICE

*Title of manuscript*: MEDUSA, a one-dimensional laser fusion code

*Authors*: J.P. Christiansen, D.E.T.F. Ashby and K.V. Roberts

*Reference*: Computer Physics Communications 7 (1974) 271

*Title of program*: MEDUSA

*Catalogue number*: ABUG

*Title of manuscript*: Form factor program for Rayleigh scattering of gamma rays by bound electrons

*Authors*: F. Smend and M. Schumacher

*Reference*: Computer Phys. Commun. 7 (1974) 389.

*Title of program*: Rayleigh form factors

*Catalogue number*: AAGY

Computer Physics Communications 9 (1975) 293–303
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# DEFORMED QUASIPARTICLE STATES IN A WOODS–SAXON POTENTIAL AND COUPLED TO ROTATIONAL STATES OF THE CORE

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Received 20 May 1975, revised version received 1 August 1975

## PROGRAM SUMMARY

*Title of program*: DEFORMED QUASIPARTICLES

*Catalogue number*: ABPF

*Computer*: IBM 360/65; *Installation*: University of Ottawa

*Operating system*: HASP

*Programming language used*: FORTRAN IV

*High speed storage required*: 23.000 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: card reader, line printer, card punch

*No. of cards in combined program and test deck*: 948

*CPC Library subprograms used*: *Catalogue number*: ABMA; *Title*: GEOMETRICAL COEFFICIENT; *Ref. in CPC* 1 (1970) 337.

*Keywords*: Nuclear, collective model, Schrodinger equation, Woods–Saxon, deformation, quasiparticle state, hexadecapole, energies, expansion coefficients.

*Nature of the problem*
The energies are calculated for the eigenstates of an odd nucleon outside a deformed core which is represented by a Woods–Saxon potential with quadrupole and hexadecapole deformations. Account is taken of pair excitations from the core with energies above that occupied by the odd nucleon. Collective excitations of the core are included, and all the rotational–particle couplings between the particle and the rotational excitations are considered, so that the complete band mixed collective spectrum of an axially symmetric permanently deformed nucleus, apart from the vibrational excitations, is generated.

*Method of solution*
The single particle bound eigenstates of a spherically symmetric Woods–Saxon potential form the basis for subsequent interaction matrix elements. This basis is obtained by radial Runge–Kutta integration. The two diagonalisations which follow add to the Hamiltonian the potential corresponding to a quadrupole and hexadecapole deformation with a derivative radial dependence, and the rotational excitations of the core. Between the two diagonalisations, a transformation to deformed quasiparticle states is made.

*Restrictions on the complexity of the problem*
The deformations are restricted to $Y_2^0$ and $Y_4^0$ shapes, with no provision for triaxial deformations or vibrational degrees of freedom. The maximum spin value which can be used in the programme is 27/2. Dimensioned space is provided for 32 states in the basis. Should the space be exceeded a warning statement is printed out. If more states in the basis or higher spin values are required, then the only modifications needed are to the array sizes within the program.

*Typical running times*
The search for each Woods–Saxon eigenstate takes about 1 sec, and the number of these states varies from about 20 near mass 100 to a maximum of 32. The diagonalisations and the quasiparticle transformation each take about 1/2 second when there are 10 states in the basis, and this time is approximately proportional to the square of the number of states.

Computer Physics Communications 10 (1975) 304–340
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# TRANSFER OF LINE RADIATION IN OPTICALLY THICK MEDIA ALLOWING FOR TRANSPORT OF EXCITATION ENERGY: THE RESONANT DOUBLET

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Received 24 September 1975

## PROGRAM SUMMARY

*Title of program*: SLAB3

*Catalogue number*: AAAH

*Computer*: CDC 6400; *Installation*: University of Colorado, computer center

*Operating system*: KRONOS

*Programming language used*: FORTRAN IV

*High speed storage required*: $61000_8 \approx 25100_{10}$

*No. of bits in a word*: 60

*Overlay structure*: 3 primary, no secondary, overlays

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, card punch

*No. of cards in combined program and test deck*: 3203

*Keywords*: Radiative transfer, resonant doublet, excitation transfer, migration of excitation, boundary layer, discrete ordinates

*Nature of physical problem*
When a confined volume of resonant vapor is excited by incident light, transfer of energy occurs both by photon scattering and by thermal motion of excited atoms with frequent excitation transfer. The random walk of a quantum of excitation may be terminated by quenching at a wall of the containing cell. This energy loss reduces the emergent radiative flux and creates a relatively under-excited boundary layer which may affect the emergent spectral profile. Our program calculates the emergent and internal radiation fields for a resonant doublet transition, the degree of excitation of the gas, and the fluxes of radiation through, and excitation into, the walls of the laboratory cell.

*Method of solution*
For each component of the doublet the equation of transfer for line radiation is coupled to the angle-dependent equation of transport for excitation, which is coupled to the other doublet component. The four coupled integro-differential equations are solved by an extension of the method of discrete ordinates. Total excitation in each transition, found by averaging the discrete streams of excited atoms, allows evaluation of the formal solution of the transfer equation for the detailed emergent radiation field.

*Restrictions on the complexity of the problem*
The cell is assumed to have planar symmetry and to be illuminated by a uniform beam impinging at a specified angle to the normal. The resonant doublet is modeled by a three-level atom in which the two closely spaced upper states are coupled only by collisional transitions and in which hyperfine structure is completely ignored. Stimulated emission is neglected, necessitating the restriction to small fractional excitation. Broadened, white and monochromatic incident beams are treated in conjunction with Doppler, Lorentz and Voigt absorption profiles, and complete frequency redistribution is assumed. Though the densities of excited states are treated as functions of flight direction, their distributions over speed are approximated by a single velocity, and excitation transfer is assumed isotropic in the laboratory frame.

*Typical running times*
For a simple case, e.g. gaussian profile with 2 streams per hemisphere and 6 frequencies representing each transition, and a monochromatic input beam, the (1, 0), (2, 0), and (3, 0) overlays required 2, 0.6, and 4 seconds, respectively (NGRID = 20; see section 3.1.9). For a more complicated case, e.g. Voigt profile with 2 streams, 20 frequencies sampling the profile for each transition and a white input beam, the (1, 0), (2, 0), and (3, 0) overlays required 19, 12, and 14 seconds respectively (NGRID = 50). The (0, 0) overlay time is negligible.

Computer Physics Communications 10 (1975) 343–367
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# MINUIT – A SYSTEM FOR FUNCTION MINIMIZATION AND ANALYSIS OF THE PARAMETER ERRORS AND CORRELATIONS

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*CH-1211 Geneva 23, Switzerland*

and

M. ROOS
*Department of Nuclear Physics, University of Helsinki,*
*Sf-00170 Helsinki, Finland*

Received 15 August 1975

## PROGRAM SUMMARY

*Title of program*: MINUIT

*Catalogue number*: ACWH

*Computer*: CDC 7600; *Installation*: CERN, Geneva, Switzerland

*Operating system*: SCOPE 2.1.2 or 2.0

*Programming language used*: ANSI FORTRAN

*High-speed storage required*: 12000 words

*Number of bits in a word*: 60

*Overlay structure*: None

*Number of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, card punch

*Number of cards in combined program and test deck*: 2600

*Keywords*: General purpose, minimization, fitting, error analysis, correlation, simplex method, variable metric method, global minimum, contours.

*Nature of physical problem*
The final stages of the analysis of experimental data often consists of determining (estimating) a certain number of physical parameters and establishing the errors (confidence regions) of these parameters. This in turn generally involves one or more stages of function minimization to determine the best parameter values and various techniques for investigating the shape of the function near the minimum to determine the errors. In this essentially statistical problem the function involved is usually a chisquare or negative log-likelihood function, however many other physical problems of a non-statistical nature, such as finding the minimum energy configuration of a molecule, can be treated using the same techniques.

*Method of solution*
We have chosen to offer the user a large number of different techniques which can be conveniently invoked by the use of command cards. For example, three different minimization algorithms are available (a Monte Carlo search [1], the simplex method of Nelder and Mead [2], and the variable metric method of Fletcher [3]) and they may be "guided" by fixing and restoring variable parameters in between minimization commands, and by putting limits on the values allowed for different parameters. Similarly, error analysis may be carried out using the covariance matrix of the function, or by calculating exact MINOS confidence intervals, or by plotting function contours. If the function is suspected of having more than one local minimum, a global minimization can be attempted using a simplified version of the algorithm of Goldstein and Price [4].

*Restriction of the complexity of the problem*
The current version is dimensioned for a maximum of 30 function parameters, of which not more than 15 may be variable.

*Typical running time*
In most cases nearly all the actual running time is spent in the

user-supplied subroutine FCN which is the function being analyzed by MINUIT. Typical applications usually require a few hundred or a few thousand function evaluations, which could in turn require much less than a second or many minutes on the CDC 7600 depending on the complexity of FCN.

*Unusual features of the problem*

MINUIT is not merely a minimization program, but is more properly a system for analysis of functions in the sense that its essential element is its structure rather than any of the algorithms that are actually implemented. This structure also allows in a very natural way the inclusion of global logic connecting the different algorithms, for example switching from one minimization method to another if the first does not converge rapidly enough.

*References*

[1] F. James, Monte Carlo for Particle Physicists (Section 6.1) in: Methods in Subnuclear Physics, Ed. M. Nikolic (Gordon and Breach Publ.) Vol. IV, Part 3.

[2] J.A. Nelder and R. Mead, Comput. J. 7 (1965) 308.

[3] R. Fletcher, Comput. J. 13 (1970) 317.

[4] A.A. Goldstein and J.F. Price, Math. Comp. 25 (1971) 569.

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Computer Physics Communications 10 (1975) 368–374
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# VIBRATIONAL ENERGIES OF $CO_2$

William C. MAGUIRE
*NASA/Goddard Space Flight Center, Greenbelt, Maryland 20771, USA*

Received 19 December 1975

## PROGRAM SUMMARY

*Title of program*: VIBOCO

*Catalogue number*: ABWC

*Computer*: IBM 360/91 or /75; *Installation*: NASA/GSFC

*Operating system*: OS/360

*Program language used*: FORTRAN IV

*High speed storage required*: 10232 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 801

*Keywords*: Molecular, spectroscopy, vibrational energy, carbon dioxide, infrared transmission, Fermi resonance, planetary, atmosphere.

*Nature of the physical problem*
Atmospheric temperature profiles and pressure values for planetary atmospheres can be determined using infrared spectra [1, 2]. Carbon dioxide bands observed in the spectra of planets are conveniently used for such calculations. Consequently, theoretical energy levels of this molecule, including various isotopic species, are required.

*Method of solution*
A molecular hamiltonian describing carbon dioxide, which is a linear triatomic, is diagonalized [3–6]. The effect of Fermi resonance is considered. The vibrational energies and rotational constants as well as mixing coefficients are obtained for levels from the ground state $(v_1, v_2, v_3; l) = (0,0,0,0)$ to the energy level $(0,24,0;24)$. Here $v_i$ is the vibrational quantum number associated with the $i$th normal mode and $l$ is the angular momentum quantum number.

*Restrictions on the complexity of the problem*
Only vibrational levels having unperturbed energy less than the energy of a state $(v_1, v_2, v_3; l) = (0,24,0;24)$ (see long write-up) are considered. For the main isotope $^{16}O^{12}C^{16}O$ with a ground-state energy at 2534.682 $cm^{-1}$ the energies range up to slightly more than 20 000 $cm^{-1}$.

*Typical running time*
A complete run for one isotope, consisting of more than 1800 energy levels, associated mixing coefficients and rotational constants takes less than a minute on an IBM 360/91.

*References*

[1] L. Pauling and E.B. Wilson, Jr., Introduction to Quantum Mechanics (McGraw-Hill, New York, 1935).
[2] G. Herzberg, Infrared and Raman Spectra (D. Van Nostrand Company, Princeton, 1945).
[3] C.P. Courtoy, Ann. de la Soc. Sci. de Bruxelles 63 (1959) 5–230.
[4] G. Amat and M. Goldsmith, J. Chem. Phys. 23 (1955) 1171–2.
[5] Gilbert Amat, Mark Goldsmith and Harald H. Nielsen, J. Chem. Phys. 24 (1956) 44–47.
[6] Charles P. Courtoy, Can. J. Phys. 35 (1957) 608–648.

Computer Physics Communication 10 (1975) 375–384
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# ROVIBRATIONAL CROSS SECTIONS FROM REACTANCE MATRICES CALCULATED IN ADIABATIC NUCLEI APPROXIMATION*

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*Baton Rouge, Louisiana 70803, USA*

Received 17 July 1975

## PROGRAM SUMMARY

*Title of program*: VIBAD

*Catalogue number*: ACWI

*Computer*: CDC 6400; *Installation*: Computing Centre, The University of Western Ontario, London, Ontario

*Operating system*: SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: 40202 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1157

*Keywords*: Molecular, scattering, electron-molecule, rotational, vibrational, cross section, reactance matrix, adiabatic nuclei approximation, Racah Coefficient.

*Nature of the physical problem*
Body frame reactance matrices obtained from elastic scattering calculations at fixed internuclear separations are transformed into laboratory frame matrices to compute differential and integral cross sections for simultaneous rotational and vibrational excitation of a molecule.

*Method of solution*
Transformation for vibrational excitation is obtained by integrating the real and imaginary parts of the body-frame $t$-matrices over internuclear separation. Vibrational wave functions are assumed to be given. The rotational transformation involves an eight-fold sum over angular momenta [1]. The summands involve $A_\lambda$-coefficients and Legendre polynominals, which are each evaluated by separate subprograms. Differential, integral, and momentum transfer cross sections are computed from the transformed $t$-matrices.

*Restriction on the complexity of the problem*
The array lengths should be adjusted to suit the user's problem and the core available on his computer. The algebraic transformations may introduce numerical inaccuracies for angular momenta $>15$, if single precision is used on a machine with shorter word length.

*Typical running time*
The sample data, comprising one energy, 8 internuclear separations, and electron orbital angular momenta $\leqslant 3$, took 14 sec CPU time.

*References*

[1] E.S. Chang and A. Temkin, Phys. Rev. Letters 23 (1969) 399;
R.J.W. Henry and E.S. Chang, Phys. Rev. A5 (1972) 276;
E.S. Chang and U. Fano, Phys. Rev. A6 (1972) 173;
A. Temkin and E.C. Sullivan, Phys. Rev. Letters 33 (1974) 1057.

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* Research supported in part by the U.S. Office of Naval Research, Contract No. N00014-69-A-0211-0004.

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Computer Physics Communications 10 (1975) 385–400

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# KINEMATICS OF THREE-BODY REACTIONS

P.A. ASSIMAKOPOULOS
*Nuclear Research Centre Demokritos, Aghia Paraskevi Attikis, Greece*

Received 11 August 1975

## PROGRAM SUMMARY

*Title of program*: PAKINE3

*Catalogue number*: ABMO

*Computer*: CDC 3300; *Installation*: N.R,C. Democritos, Athens

*Operating system*: MASTER 4.0

*Program language used*: FORTRAN IV

*High speed storage required*: 8720 words

*No. of bits in a word*: 24

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 362

*Keywords*: Nuclear, kinematics, reaction, three-body, final-state interaction, recoil centre-of-mass system, angular distribution.

*Nature of physical problem*
The Long Write-up summarizes the expressions for evaluating the kinematic variables in reactions of the form $A + B \rightarrow a_1 + a_2 + a_3$. These variables include the kinetic energy of particles in the final state, the relative final state interaction energy for each pair, the corresponding centre-of-mass angles and angles in the centre-of-mass system of an interacting pair. The various centre of mass systems employed here are discussed by Swann [1]. Program PAKINE3 evaluates all these kinematic variables and is an extension of a program described in ref. [2]. Program PAKIPLOT produces on the lineprinter a 64 × 64 channel plot of the kinematic locus for the reaction.

## PROGRAM SUMMARY

*Title of program*: PAKIPLOT

*Catalogue number*: ABMP

*Computer*: CDC 3300; *Installation*: N.R.C. Demokritos, Athens

*Operating system*: MASTER 4.0

*Program language used*: FORTRAN IV

*High speed storage required*: 8503 words

*No. of bits in a word*: 24

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 213

*Restriction on the complexity of the problem*
The kinematics is worked out in the non-relativistic limit and for a coplanar geometry.

*Typical running time*
PAKINE3 calculates all the kinematic variables for six pairs of angles of detection in 1 min. PAKIPLOT calculates and plots on the lineprinter the kinematic loci for five simultaneou reactions in $\frac{1}{2}$ min.

*References*

[1] P. Swan, Rev. Mod. Phys. 37 (1963) 336.
[2] P. Assimakopoulos, Programme No. 3, NRCD/IDR, 1965.

Computer Physics Communications 10 (1975) 401–420
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# PATIWEN – A CODE FOR COULOMB–NUCLEAR INTERFERENCE CALCULATIONS *

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and

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Received 25 July 1975; revised manuscript received 19 December 1975

## PROGRAM SUMMARY

*Title of program*: PATIWEN

*Catalogue number*: ABPD

| *Computer*: | *Installation*: |
|---|---|
| IBM 370/165 | Daresbury Nuclear Physics Laboratory, Cheshire, U.K. |
| CDC 7600 | UMRCC, Manchester |

*Operating system*: OSRLSE 21

*Program language used*: FORTRAN IV

*High speed storage required*: 344 K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Line printer, card reader

*No. of cards in combined program and test deck*: 1256

*CPC Library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ABPC | RCWFN | 8 (1974) 377 |
| ABPC 0001<br>(optional) | RCWFF | to be published |

*Keywords*: Nuclear, electric multipole, Coulomb excitation, differential, cross sections, inelastic, scattering, radial integrals, partial-wave expansion, Eλ Coulomb matrix elements, continued fractions.

*Nature of the physical problem*
The program PATIWEN calculates the differential and total cross sections for inelastic scattering of a structureless charged particle interacting via an electric multipole of order E2–E6 with a nuclear system. It is also designed to accept nuclear matrix elements (up to 150 partial waves) from any conventional DWBA program [1] and to complete a full Coulomb–nuclear interference calculation. A subroutine generates radial matrix elements of the type $\int_a^b \mathrm{d}r\, u_l(kr)\, r^{-\lambda-1}\, u_{l'}(k'r)$, where $\lambda \geq 1$ and where $u_l(kr)$ is a combination of Coulomb wavefunctions, for positive, negative and zero values of the Sommerfeld parameter, $\eta$.

*Method of solution*
The numerical calculation closely follows the quantum-mechanical theory of nuclear and Coulomb excitations in the distorted-wave Born approximation [2]. The projectile is assumed to be a point charge. The radial matrix elements are integrated by the gaussian quadrature [3] technique. This represents an attractive procedure as the Coulomb functions needed for the integrand can be calculated independently at any radius using subroutine RCWFN [4]. An adaptation [5] of RCWFN which requires less array space can be used.

*Restriction on the complexity of the problem*
The calculation is non-relativistic and is dimensioned for 600 partial waves; more can be included if necessary. There is no inherent restriction to the scattering of like charges, although only this case has been tested.

---

* Work supported by the United Kingdom Science Research Council and the U.S. Energy Research and Development Administration.

*Typical running time*

The running time depends directly on the integration range and the number of partial waves, i.e. on $\rho L$. For a typical heavy-ion E2 case with $\rho = 800$ ($r = 250$ fm) and $L = 500$ the running time is about 3 minutes, while for the E3 test case $\rho = 400$ ($r = 250$ fm) and $L = 145$ the time is 50 sec. These times are central processor times for the IBM 370/165 computer; they could be drastically reduced by exploiting various recurrence relations among the Coulomb matrix elements.

*References*

[1] P.D. Kunz, University of Colorado, DWUCK, unpublished; T. Tamura, W.R. Coker and F. Rybicki, Computer Phys. Commun. 2 (1971) 94.

[2] L.C. Biedenharn and P.J. Brussard, *Coulomb Excitation* (Oxford: Clarendon Press, 1965);
B. Buck, Phys. Rev. 127 (1962) 940; 130 (1963) 172;
R.H. Bassel, G.R. Satchler, R.M. Drisko and E. Rost, Phys. Rev. 128 (1962) 2693;
K. Alder, A. Bohr, T. Huus, B. Mottelson and A. Winther, Rev. Mod. Phys. 28 (1956) 432.

[3] P.J. Davis and I. Polonsky, *Handbook of Mathematical Functions*, ed. M, Abramowitz and I.A. Stegun (Dover Publications Inc., N.Y., 1964) p. 875.

[4] A.R. Barnett, D.H. Feng, J.W. Steed and L.J.B. Goldfarb, Computer Phys. Commun. 8 (1974) 377.

[5] A.R. Barnett, Computer Phys. Commun., to be published.

Computer Physics Communications 10 (1975) 421–433
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# A FINITE-ELEMENT PROGRAM PACKAGE FOR MAGNETOTELLURIC MODELLING

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Received 20 March 1975

## PROGRAM SUMMARY

*Title of program*: H-PARALLEL FEMT-2D

*Catalogue number*: ACSG

*Computers*: IBM 360/75, IBM 370/158; *Installation*: McGill University Computing Centre, Montreal, Quebec, Canada

*Operating system*: OS/360 with HASP II

*Programming language used*: FORTRAN IV

*High speed storage required*: 50K words

*No. of bits in a word*: 32

*Overlay structure*: Overlaid

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 4109

*CPC Library subprograms used*: (optional); *Catalogue number*: ACSJ; *Title*: ZFORMATS; *Ref. in CPC*: this paper.

*Keywords*: Geophysics, magnetotelluric, finite element, Laplace, Helmholtz, *H*-parallel, *H*-polarization, *E*-parallel, *E*-polarization, Cuthill–McKee, sparse matrices.

*Nature of physical problem*
Telluric and magnetotelluric response over two-dimensional resistivity anomalies and topographic variation in the *H*-parallel case.

*Method of solution*
The high-order triangular finite element method is used with polynomials of degree up to six. The resultant linear system of equations is not solved by an iterative process; rather, the complex symmetric positive-definite coefficient matrix is factorized into $LDL^T$. The generation of nodes is mostly automatic and is followed by reordering according to the reverse Cuthill–McKee algorithm to improve matrix profile and thus greatly reduce storage requirements. Surface electric field values are computed with the matrix representation of the normal derivative operator.

*Restrictions on the complexity of the problem*
The usual assumptions of magnetotelluric modelling are assumed [1]. Only geological structures having infinite length in one direction are treated. It is assumed that all boundaries within the problem region can be well approximated by straightline segments.

*Typical running times*
The execution times are greatly problem-dependent. The sample problem of a vertical fault described in the long write-up and involving the solution of a complex linear system of 235 unknowns required 25 seconds in total CPU time on the IBM 360/75 computer.

*Unusual features of the program*
Data in the BLOCK DATA BLOCK1 of the program are punched in Z format, a feature of the IBM FORTRAN IV. This BLOCK DATA can be generated in other formats using the program ZFORMATS described in this paper and which must be suitably modified.

*References*
[1] L. Cagniard, Geophysics 18 (1953) 605–635.
[2] P. Silvester, Intern. J. Eng. Sci. 7 (1969) 849–861.

## PROGRAM SUMMARY

*Title of program*: E-PARALLEL FEMT-2D

*Catalogue number*: ACSH

*Computers*: IBM 360/75, IBM 370/158; *Installation*: McGill University Computing Centre, Montreal, Quebec, Canada

*Operating system*: OS/360 with HASP II

*Programming language used*: FORTRAN IV

*High speed storage required*: 75 words

*No. of bits in a word*: 32

*Overlay structure*: Overlaid

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 6245

*CPC Library subprograms used*: (optional); *Catalogue number*: ACSJ; *Title*: ZFORMATS; *Ref. in CPC*: this paper.

*Keywords*: Geophysics, magnetotelluric, finite element, Laplace, Helmholtz, $H$-parallel, $H$-polarization, $E$-parallel, $E$-polarization, Cuthill–McKee, sparse matrices.

*Nature of the problem*
Telluric and magnetotelluric response over two-dimensional resistivity anomalies and topographic variations in the $E$-parallel case.

*Method of solution*
In addition to the features found in the program H-PARALLEL FEMT-2D a recursive approach has been developed to expand the region in space which will consist, a posteriori, of a problem-dependent number of identical air strips. Field computations are restricted to nodes on or below the ground surface. Thus storage requirements are relatively not much larger than those of the $H$-parallel case.

*Typical running times*
The same vertical fault treated in the $H$-parallel case has now 264 free nodes. It requires three air strips to yield a relative variation smaller than 1% in the values of the apparent resistivity. The total CPU time is 53 seconds.

## PROGRAM SUMMARY

*Title of program*: ZFORMATS

*Catalogue number*: ACSJ

*Computers*: IBM 360/75, IBM 370/158; *Installation*: McGill University Computing Centre, Montreal, Quebec, Canada

*Operating system*: OS/360 with HASP II

*Programming language used*: FORTRAN IV

*High speed storage required*: 25K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: card reader, line printer, card punch

*No. of cards in combined program and test deck*: 585

*Purpose of the program*
This program reads in the finite element matrices described in [1] in integer form and punches out the complete block data subprogram BLOCK1 containing these matrices in Z-format as listed in the programs H-PARALLEL FEMT-2D and E-PARALLEL FEMT-2D. Users of computers other than the IBM 360 or 370 series will have to modify output format statements in ZFORMATS and generate a new BLOCK1 compatible with their compiler.

*Typical running times*
On the IBM 360/75 computer it takes 10 seconds of CPU time to run ZFORMATS.

*Reference*

[1] P. Silvester, Intern. J. Eng. Sci. 7 (1969) 849–861.

Computer Physics Communications 10 (1975) 434–435
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## ERRATUM NOTICE

*Title of manuscript*: CIV3 – A general program to calculate configuration interaction wave function and electric dipole oscillator strengths

*Author*: A. Hibbert

*Reference*: Computer Phys. Commun. 9 (1975) 141

*Title of program*: CIV3 A GENERAL C.I. PROGRAM

*Catalogue number*: AAKM

*Title of manuscript*: A non-relativistic scf atomic program to compute one-electron energies, total energies and Slater integrals

*Authors*: J.H. Wood and M. Boring

*Reference*: Computer Phys. Commun. 7 (1974) 73

*Title of Program*: HERSKLZARE

## ERRATUM

Ajit J. Thakkar and Vedene H. Smith, Jr., Ring and other contributions to the higher virial coefficients, Computer Phys. Commun. 10 (1975) 80–85.

The number in the first row and last column of table 3 should be −0.0975 and not 0.0975.

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Computer Physics Communications 11 (1976) 5–25
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# TRANAL – A PROGRAM FOR THE TRANSLATION OF SYMBOLIC ALGOL I INTO SYMBOLIC ALGOL II

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Received 19 December 1975

## PROGRAM SUMMARY

*Title of program*: TRANAL

*Catalogue number*: ABUN

*Computer*: ICL 4–70; *Installation*: UKAEA Culham Laboratory

*Operating system*: ICL Multijob

*Programming languages used*: ECMA Algol, with ICL System 4 I/O procedures

*High-speed store required*: 42976 bytes + stack

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes used*: None

*Other peripherals used*: 2 line files for output, card reader

*No. of cards in combined program and test deck*: 700

*Keywords*: Symbolic Algol, translator, magnetohydrodynamics, vector notation, general purpose, utility.

*Nature of problem*
Two symbolic styles of Algol 60 programming have previously been developed for the expression of partial differential equations in vector form: SAI [1] which solves the equations directly but executes slowly because of the large number of nested procedure calls involved and SA II [2] which is used to generate an optimized version of the program in a chosen target language. Conversion from SAI to SAII has previously been carried out by hand and the present program TRANAL is intended to perform this process automatically. It is written in Algol 60 and illustrates the usefulness of Algol for the manipulation of physics equations. The main SA I & II program packages will be published in due course.

*Method of solution*
Each SA I equation is read character by character and converted by recursive syntax analysis into a tree structure. It is then output in SA II form by an appropriate set of rules.

*Restrictions on the complexity of the problem*
The number and complexity of the equations can be increased by changing the symbolic parameters in #1.2 of the program. TRANAL is written in ECMA Algol 60 and conversion to most computer systems should only entail changing a few system-dependent I/O procedures in #6. The operators currently allowed are the basic operators +, –, *, / together with arbitrary unary and binary function operators such as CURL(A) and CROSS(A,B). Limited error diagnostics are provided, and the working of the program can be examined on a second output channel by including the symbol '$' in the input deck.

*Typical running time*
With diagnostics switched off, the Test Run requires 3½ sec on the Culham ICL 4–70.

*References*

[1] K.V. Roberts and J.P. Boris, J. Comp. Phys. 8 (1971) 83.
[2] M. Petravic, G. Kuo–Petravic and K.V. Roberts, J. Comp. Phys. 10 (1972) 503.

Computer Physics Communications 11 (1976) 27–35
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# A PROGRAM TO CALCULATE GREEN'S FUNCTIONS*

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Received 10 February 1976

## PROGRAM SUMMARY

*Title of program*: GRN1

*Catalogue number*: ACWN

*Computer*: CDC 6400; *Installation*: Computing Centre, The University of Western Ontario, London, Ontario.

*Operating system*: SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: 42477 words.

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: card reader, line printer.

*No. of cards in combined program and test deck*: 1218

*Keywords*: General purpose, Green's functions, Ricatti–Bessel, modified Ricatti–Bessel, Coulomb function, Whittaker functions, scattering.

*Nature of the physical problem*
Regular and irregular solutions to a one-dimensional differential equation are obtained for the cases where the potential includes a Coulomb term and/or a centrifugal barrier, and for positive or negative energies. These Green's function solutions are necessary, for example, in the solution of a scattering problem by the non-iterative integral equation method [1].

*Method of solution*
A power series expansion for small values of the radial distance is used for both the regular and irregular solutions [2]. When the amplitude of the solutions are approximately the same, the power series is replaced by a Numerov integration method, by which the solutions are generated outwards to large values of the radial distance. For the case of negative energy, the irregular solution is obtained at large radial values by an asymptotic expansion [2] and is generated inwards by a Numerov method.

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* Research on neutral atoms supported in part by the U.S. Office of Naval Research, Contract No. N00014-76-C-0041; research on ions supported in part by the U.S. Energy Research and Development Administration, Division of Physical Research, Contract No. AT-(40-1)-4881.

‡ Supported in part by the National Aeronautics and Space Administration through contract NSG-901.

*Restrictions on the complexity of the program*

The order of the Green's functions is restricted to $l \leqslant 24$. The arrays used in the storage of the power series coefficients must be increased for $l > 24$. The program can be used for all positive and negative energies except for energies which can be written in the form $E = -n^{-2}$, where $n$ is a positive integer. Numerical inaccuracies will result if the program is used in single precision on a 32 bit/word computer.

*References*

[1] E.R. Smith and R.J.W. Henry, Phys. Rev. A7, (1973) 1585.

[2] M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions (U.S. Department Commerce, N.B.S., Applied Mathematics Series 55, 1965).

Computer Physics Communications 11 (1976) 37–48
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# ANNA: AN INTERACTIVE PROGRAM FOR ANALYSIS OF ONE-DIMENSIONAL PULSE-HEIGHT SPECTRA

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Received 11 August 1975

## PROGRAM SUMMARY

*Title of program*: ANNA

*Catalogue number*: ABMN

| *Computer*: | *Installation*: |
|---|---|
| PDP-15 | N.R.C. Demokritos, Athens |

*Operating system*: ADSS-15, KM15 V5A

*Programming language used*: FORTRAN IV, MACRO-15

*High speed storage required*: 16K words

*No. of bits in a word*: 18

*Overlay structure*: None

*No. of magnetic tapes required*: One DECTape (optional)

*Other peripherals used*: teletype, paper tape read/punch, visual display screen with lightpen (VR15-CL)

*No. of cards in combined program and test deck*: 1124

*Keywords*: Nuclear, analysis, spectrum, gamma-ray, spectoscopy, charged particle, spectrum stripping, peak analysis, gaussian fit, background fit.

*Nature of physical problem*
The program is an aid in the analysis of one-dimensional nuclear data (e.g., $\gamma$-ray spectra). It can however be used in all cases, where histogram-type data with Poisson Statistics is analyzed

*Method of solution*
Interactive computation is employed. A portion of the data is displayed on a CRT-screen, the area of interest is indicated with the lightpen and various processing commands are executed by changing the state of the ACCUMULATOR SWITCHES. A log of all operations and results is printed on the teletype. Commands already programmed are: Control of I/O, polynomial fit to background, centroid and area of peaks, multiple (1 to 3) gaussian fit. The correct statistical errors are computed and printed along with the parameter values.

*Restriction on the complexity of the problem*
A symmetric gaussian is fitted to the data. Thus, fits to multiple peaks with high or low energy tails should be accepted with some caution.

*Typical running time*
The program is interactive and runs until stopped by the user/operator. The longest single operation recorded up to now was a double gaussian fit to a structure extending over 128 channels which took four minutes (five iterations).

*Unusual features of the program*
The program is designed to run on a PDP-15 computer with the minimum of peripheral equipment, notably without a card reader or lineprinter – as is usually the case for such computers employed mainly for on-line data acquisition. (If however a lineprinter is available it can be readily employed by assigning prior to execution I/O device #2 to the lineprinter. In such a case a complete log of the operations will be kept on the lineprinter). Due to this restriction the source program is available in the form of a DECTape. The DECTape contains all source (SRC) and Binary (BIN) programs, as well as the appropriate XCT and XCU files, compiled under the CHAIN system for single-command execution. The source program is also available as a card deck.

Computer Physics Communications 11 (1976) 49–55
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# DIPOLE AND OVERLAP INTEGRALS BETWEEN SLATER-TYPE FUNCTIONS AND CONTINUUM COULOMB FUNCTIONS

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and

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Received 2 December 1975

## PROGRAM SUMMARY

*Title of program*: ONEINT

*Catalogue number*: ABWB

| *Computer*: | *Installation*: |
|---|---|
| CDC 6400 | Center for Astrophysics, Cambridge, Mass., USA |

*Operating system or monitor under which the program is executed*: SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: 50 000 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used:* Scratch disk space, card reader, line printer

*No. of cards in combined program and test deck*: 839

*Keywords*:
Molecular physics quantum chemistry, theoretical methods, dipole integral, coulomb, molecular electronic continuum, photoionization, Slater-type functions

*Nature of physical problem*
Two-center one-electron dipole and overlap integrals between Slater-type functions and Coulomb continuum functions can be useful in computing molecular photoionization cross sections [1]. The Slater functions are assumed to be centered on the nuclei, A and B, and the Coulomb function can be centered at nucleus A or any point between A and B.

*Method of solution*
The integrals are evaluated numerically using a one-center expansion of Slater-type functions at the origin of the Coulomb function.

*Restrictions on the complexity of the problem*
The maximum number of Slater-type functions is 50. Only one value of the quantum numbers $l$ and $m$ for the Coulomb function is allowed, although up to 20 Coulomb energies can be calculated in a single run.

*Typical running time*
Compile time 7 seconds; one center expansion requires 10 seconds and for each Coulomb energy approximately 0.1 second per integral is required.

*Unusual features of the program*
The more Coulomb energies that are computed in a given run, the more time-efficient the overall integral program becomes.

*Reference*
[1] A.L. Ford, K.K. Docken and A. Dalgarno, Ap. J., 195 (1975) 819.

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# SELF-CONSISTENT FIELD HARTREE–FOCK PROGRAM FOR ATOMS

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and

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*and*
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Received 17 July 1975

## PROGRAM SUMMARY

*Title of program*: ATOMIC SCF HARTREE-FOCK

*Catalogue number*: AAKQ

*Computer*: CDC 3600; *Installation*: Boris Kidrich Institute

*Operating system*: Tape SCOPE 6.3

*Programming language used*: ALGOL 60

*High speed storage required*: 32K words

*No. of bits in a word*: 48

*Overlay structure*: None

*No. of magnetic tapes required*: One or none

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 428

*Keywords*: Atomic, structure, energy level, wave functions, independent-particle approximation, single-particle model, Hartree–Fock, (many-) electron correlations, electron configuration, single-configuration approximation, atomic shell, *nl*-(sub) shell, self-consistent field, iteration convergency acceleration, Numerov method, chasing method, Gauss elimination method without pivoting, energy eigenvalue adjustment.

*Nature of physical problem*
The present program calculates one-electron radial wave functions and energy eigenvalues by solving non-relativistic single-configuration Hartree–Fock (HF) equations for bound states of an atom [1].

*Method of solution*
HF equations are solved by iterations [1] until self-consistency is achieved. To stabilize the iteration process and to accelerate its convergence special procedures are applied.

The differential equation, appearing in the iteration process, is solved using the Numerov method [1]. The energy eigenvalue is so adjusted that the corresponding radial function satisfies the boundary conditions and has the required number of nodes.

*Restrictions on the complexity of the problem*
Off-diagonal parameters, which vanish for closed *nl*-subshells [1], are neglected in the present program. Therefore, the program could be used for configurations with the majority, if not all, closed *nl*-subshells, e.g., for the ground state configurations where these parameters and very small [2].

For certain configurations with excited single-electron d or f states (like e.g., $_{20}$Ca 4s4d($^3$D)) instabilities in solving the corresponding equation can occur, which prevent a solution being obtained.

*Typical running time*
For the ground state configuration of nitrogen $1s^2 2s^2 2p^3 (^4S)$,

with 700 integration points of the independent variable, the total running time including compilation amounts to about 10 minutes on a CDC 3600 computer with all peripherals connected on-line, and with the operating system (SCOPE) on a magnetic tape.

*Unusual features of the program*

The present program is designed so that the results can be used directly as input data for another program [3], which calculates excited discrete and continuum states. Consequently, the independent variable in both of these programs is related to the radial variable by the transformation [4] $x = \alpha r + \beta \ln r$, which for excited, especially continuum states, behaves suitably at large values of $r$, while at small values of $r$ it has the usual logarithmic behaviour.

*References*

[1] D.R. Hartree, The calculation of atomic structures (John Wiley, New York, 1957).

[2] J.B. Mann, Atomic structure calculations I. Hartree–Fock energy results for the element hydrogen to lawrencium. Los-Alamos Scientific Laboratory report LA-3690 (1967).

[3] L.V. Chernysheva, N.A. Cherepkov and V. Radojević, Frozen core Hartree–Fock program for atomic single-electron discrete and continuous states, to be submitted for publication to Computer Phys. Commun.

[4] V.F. Bratcev, The tables of atomic wave functions (Nauka, Moscow, 1965 – in Russian).

Computer Physics Communications 11 (1976) 75–93
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# A PROGRAM FOR CALCULATING GAMMA–GAMMA DIRECTIONAL CORRELATION COEFFICIENTS AND MIXING RATIOS

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Received 8 July 1975

## PROGRAM SUMMARY

*Title of program*: ANGCOR

*Catalogue number*: ABPG

| *Computer*: | *Installation*: |
|---|---|
| CDC 7600, 6600 | Lawrence Livermore Laboratory<br>Livermore, California, USA. |

*Operating system*: FLOE

*Programming language used*: FORTRAN IV

*High-speed storage required*: 25 344 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, teletypewriter, disc, CRT data display

*No. of cards combined program and test deck*: 1361

*Keywords*: Nuclear, spectroscopy, directional, correlation, mixing ratios, solid-angle corrections, orientation, directional distribution, chi-square, F-coefficient, Clebsch–Gordan, Legendre polynomial, multipolarity, Wigner, 3–*j*, 6–*j*, symbols, experiment, admixture.

*Nature of the physical problem*
Conservation of angular momentum governs the multipolarity of electromagnetic transitions between nuclear excited states. In certain cases a mixture of two multipolarities may occur in a single transition. The amount of mixing, i.e., the mixing ratio, is determined by the structure of the nuclear levels involved. By accurately measuring the directional correlation between two transitions and comparing it with several theoretically expected correlations, the most probable mixing ratio can be determined.

*Method of solution*
The program has two modes of operation: in the first mode, directional correlation coefficients are determined by least-squares fits to the experimental data with second- and fourth-order Legendre polynomials having only even terms. The coefficients are then corrected for the experimental finite solid angles. For each spin sequence entered, a chi-square value is calculated for 49 possible values of each transition mixing ratio. The printout appears as a 49 by 49 point grid which resembles a contour map. A study of several of these printouts allows the user to qualitatively determine possible spin sequences and mixing ratios. Mode II, the data simulation mode, calculates a set of directional correlation coefficients from spins and mixing ratios entered, corrects for solid angle, and calculates a set of angular correlation data normalized to $A_0 = 10\,000$. The required inputs are spin assignments for the three levels, mixing ratios of the transitions, and the experimental solid-angle corrections. The second mode allows tests of the program or examination of results for given spin sequences and mixing ratios. An option in both modes magnifies any section of the $\chi^2$ grid.

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* Research supported in part by the U.S. Energy Research & Development Administration.

** Research supported by Fannie and John Hertz Foundation.

*Restrictions on the complexity of the program*
Input must be ten angles or fewer. Correlations are limited to to successive gamma-ray cascades.

Computer Physics Communications 11 (1976) 95–112
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# DWPI: A COMPUTER PROGRAM TO CALCULATE THE INELASTIC SCATTERING OF PIONS FROM NUCLEI*

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Received 19 August 1975

## PROGRAM SUMMARY

*Title of program*: DWPI

*Catalogue number*: ABIG

*Computer*: UNIVAC 1108; *Installation*: Computer Center, Carnegie–Mellon Univ., Pittsburgh, Pa. 15213, USA. Program has also run on CDC 6600, 7600, IBM 360/67, DEC PDP-10

*Operating system*: UNIVAC EXEC II

*Program language used*: FORTRAN IV

*High speed storage required*: $43138_{10}$ words

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader and line printer

*No. of cards in combined program and test deck*: 890

*CPC Library subprograms used*: Cat. no: ABCJ; *Title*: PIRK; *Ref. in CPC*: 8 (1974) 130.

*Keywords*: Nuclear, pion, inelastic, scattering, distorted wave, impulse approximation, optical model, angular distribution, Klein–Gordon, cross section.

*Method of solution*
Angular distributions for the inelastic scattering of pions are generated using the distorted wave impulse approximation (DWIA). The cross section for a given transition is calculated by summing a partial wave expansion. The $T$-matrix elements are calculated using distorted pion waves from the program PIRK, and therefore include elastic scattering to all orders. The excitation is treated in first order only. Several optical potentials and nuclear densities are available in the program. The transition form factor may be uncoupled from the ground-state density. Coulomb excitation, which interferes coherently with the strong interaction, is a program option.

*Restrictions on the complexity of the program*
A maximum of 30 partial waves (500 mesh points each) in the incoming channel can be used without changing the program. The maximum angular momentum transfer is $\lambda \leqslant 5$. The nuclear form factor is from a collective model. The program presently includes only a restricted class of non-local potentials; other types of non-localities may be of physical interest.

*Typical running time*
This depends on the number of partial waves, the number of mesh points, the value of transferred angular momentum $\lambda$, and the ground state spin. The test case given requires 28 seconds on the Univac 1108 (15 partial waves, 100 integration steps per partial wave, $I = 0, I' = 2$).

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* Work supported by the ERDA (Contract AT(11-1)3244) and the NSF.

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# MATRIX ELEMENTS OF THE REACTION MATRIX IN FINITE NUCLEI*

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Received 15 August 1975

## PROGRAM SUMMARY

*Title of program*: REFERENCE REACTION MATRIX

*Catalogue number*: ABIE

*Computer*: IBM 360/65; *Installation*: University of Ottawa, Ottawa, Canada

*Operating system*: HASP 0S/360 Level 21.8

*Programming language used*: Fortran IV

*High speed storage required*: 31K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, card punch

*No. of cards in combined program and test deck*: 1000

*CPC Library subprograms used (for data)*:

*Catalogue number*: ABIF; *title*: REACTION MATRIX; *Ref. in CPC*: this paper

*Keywords*: Nuclear, reference reaction matrix, finite nuclei

## PROGRAM SUMMARY

*Title of program*: REACTION MATRIX

*Catalogue number*: ABIF

*Computer*: IBM 360/65; *Installation:* University of Ottawa, Ottawa, Canada

*Operating system*: HASP 0S/360 Level 21.8

*Programming language used*: Fortran IV

*High speed storage required*: 52.5 K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: 1 (optional)

*Other peripherals used*: Card reader, line printer, card punch, magnetic disk (optional)

*No. of cards in combined program and test deck*: 2053

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* Work supported in part by the National Research Council of Canada.

*CPC Library subprogram used (for data)*:
*Catalogue number*: ABIE; *title*: REFERENCE REACTION MATRIX; *Ref. in CPC*: this paper.

*Keywords*: Nuclear, reaction matrix, finite nuclei

*Nature of the problem*
Matrix elements of the reaction matrix in finite nuclei are computed in the relative center-of-mass (RCM) harmonic-oscillator representation. A harmonic oscillator Pauli operator is employed together with purely kinetic particle states. The approach used follows that of Sauer [1]. The Reid soft-core potential [2] is employed in the code discussed.

*Method of solution*
A reference reaction matrix is first computed by matrix inversion, and harmonic-oscillator matrix elements of this evaluated by a double integration. The reaction matrix elements can then be determined by solving a set of linear algebraic equations.

*Restrictions on the complexity of the problem*
Matrix inversion is used to solve for the reference reaction matrix, as well as in the evaluation of the operators involved in the determination of the reaction matrix. The maximum dimension allowed is 16, However very good results are obtained using a dimension of 6.

*Unusual features of the program*
During the first run of ABIF (REACTION MATRIX), data is output for use with ABIE (REFERENCE REACTION MATRIX), which in turn outputs required data for subsequent runs of ABIF.

*Typical running times*
The run of REACTION MATRIX to obtain a punched data deck takes approximately 5 seconds for each 10 matrix elements. REFERENCE REACTION MATRIX requires roughly 10 seconds for each 4 $T$-matrix elements. This figure was obtained from the test run. If a large number of elements are computed, this figure improves, as more use is made of stored intermediate results. REACTION MATRIX needs about 10 seconds for each 5 matrix elements. Both these times are exclusive of compile times

*References*

[1] P.U. Sauer, Nucl. Phys. A150 (1970) 467.
[2] R.V. Reid, Ann. of Phys. (N.Y.) 50 (1968) 411.

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Computer Physics Communications 11 (1976) 125–140
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# ADAPTATION OF CIV3 TO EVALUATE HYPERFINE STRUCTURE

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Received 5 January 1976

## ADAPTATION SUMMARY

*Title of adaptation:* ADAPT CIV3 FOR HFS

*Adaptation number*: 0001

*Reference to original program*:
*Catalogue number*: AAKM; *Title*: CIV3 A GENERAL C.I. PROGRAM; *Ref. in CPC*: 9 (1975) 141.

*Author of original program*: A. Hibbert

*No. of cards required to effect adaptation (including directive cards)*: 880

*CPC Library subprograms used*:

| *Catal. number* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACQB | P SHELL C.F.P. | 1 (1969) 15 |
| ACRN | A NEW D SHELL CFP | 6 (1973) 88 |
| AAGD | NJSYM | 1 (1970) 241,<br>2 (1971) 173 |
| AAGD0001 | ADAPT NJSYM FOR WEIGHTS | 2 (1971) 180 |
| AAGD0002 | ADAPT TO INTEGER ARITHMETIC | 5 (1973) 161 |
| ACQV | WEIGHTS NEW VERSION | 2 (1971) 180,<br>6 (1973) 59 |
| ACQV0001 | ADAPT WEIGHTS FOR ONE-ELECT | 7 (1974) 318 |
| ACQV0002 | ADAPT TO TEST CONFIG DATA | 8 (1974) 329 |
| AAKF | REDUCED TENSOR MATRIX ELEMENTS | 6 (1973) 132,<br>9 (1975) 268 |
| AAKF0001 | ADAPT TENSOR FOR PRODUCTS | This paper |

*Additional keywords*: Hyperfine structure

*Nature of physical problem*
The adaptation effects the use of configuration interaction wave functions generated by the original program in the evaluation of magnetic dipole and electric quadrupole hyperfine structure parameters and energy corrections. Parameters both diagonal and off-diagonal in $J$ are considered.

*Restrictions on the complexity of the problem*
Same as for the original program

*Typical running time*
Two new data sets are added to the original eight. The additional time for Case 9 (lithium $^2P$) and Case 10 (oxygen $^3P$) is 8 minutes (on an ICL 1906A), of which 5 minutes is used in the evaluation of the wave functions.

---

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## ADAPTATION SUMMARY

*Title of adaptation*: ADAPT TENSOR FOR PRODUCTS

*Adaptation number*: 0001

*Reference to original program*:
*Catalogue number*: AAKF; *Title*: REDUCED TENSOR MATRIX ELEMENTS; *Ref. in CPC*: 6 (1973) 132

*Authors of original program*: W.D. Robb

*No. of cards required to effect adaptation (including directive cards)*: 55

*CPC Library subprograms used*: Same as original program

*Additional keywords*: Tensor products

*Nature of physical problem*
The program TENSOR evaluates the reduced matrix elements of a one-particle tensor operator between arbitrarily $L-S$-coupled configurations. The present adaptation extends its use to evaluate the matrix elements (not reduced) of a simple of two tensors, one spin-dependent, the other other space-dependent. Product of tensors are required in magnetic hyperfine structure calculations by adaptation 0001 of AAKM.

Computer Physics Communications 11 (1976) 141–142
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# RCWFF – A MODIFICATION OF THE REAL COULOMB WAVEFUNCTION PROGRAM RCWFN

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Received 5 February 1976

## ADAPTATION SUMMARY

*Title of adaptation*: RCWFF

*Adaptation number*: ABPC0001

*Reference to original program*:
*Catalogue number*: ABPC; *Title*: RCWFN; *Ref.* in CPC: 8(1974)377

*Authors of original program*: A.R. Barnett, D.H. Feng, J.W. Steed and L.J.B. Goldfarb

*No. of cards required to effect adaptation (including directive cards)*: 74

*Nature of the physical problem*
The subroutine RCWFF calculates Coulomb wavefunctions and returns (1) $F_l(\eta,\rho)$; or (2) $F_l(\eta,\rho)$ and $G_l(\eta,\rho)$; or (3) $F_l(\eta,\rho)$, $G_l(\eta,\rho)$, $F_l'(\eta,\rho)$ and $G_l'(\eta,\rho)$, where the primes denote d/d$r$ and $\rho = kr$. When in use as under (3) it is identical with subroutine RCWFN [1] and the range of values, method of solution, restrictions, and timing remain the same. When used as in (1) or (2) the program is somewhat faster, since less calculation and normalisation is required, and it requires no array space for the unwanted quantities.

The subroutine has been incorporated into the DWBA program PATIWEN [2,3] which is used to evaluate light-ion and heavy-ion Coulomb nuclear interference in inelastic scattering. For these calculations real Coulomb matrix elements of the form

$$\int_a^b F_l(\eta,kr)\, r^{-\lambda-1}\, F_{l'}(\eta',k'r)\, \mathrm{d}r$$

are required for the bulk of the calculation and so RCWFF is called as in (1) above.

*Typical running time*
The time saving depends on the relative time spent in evaluating the two continued fractions compared with the calculation of the unwanted quantities: when only $F_l(\eta,\rho)$ is required savings of up to 30% have been found, if the parameters are in the range normal for heavy-ion physics calculations.

*Test run*
The testing routine has been modified to call RCWFF three times for the different modes of operation. The results are displayed one after the other in the order of the original test of RCWFN. The first few lines of output are reproduced below to illustrate the format.

*References*

[1] A.R. Barnett, D.H. Feng, J.W. Steed and L.J.B. Goldfarb, Computer Phys. Commun. 8 (1974) 377.
[2] D.H. Feng and A.R. Barnett, Computer Phys. Commun. 10 (1975) 401.
[3] A.R. Barnett, D.H. Feng and L.J.B. Goldfarb, Phys. Rev. C 13 (1976) no. 3.

Computer Physics Communications 11 (1976) 199–209
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# CONVERTER OF FORTRAN FORMAT AND DATA STATEMENTS TO STANDARD FORM

M. SALEM *
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Received 16 June 1975, revised manuscript received 23 February 1976

## PROGRAM SUMMARY

*Title of program*: FORMAT AND DATA CONVERTER

*Catalogue number*: ACWP

*Computer*: IBM 360/65; *Installation*: University College London Computer Centre

*Operating system*: OS

*Program language used*: FORTRAN IV

*High speed storage required*: 22000 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, card punch

*No. of cards in combined program and test deck*: 1304

*Keywords*: General purpose, utility, FORMAT, DATA, ANSI, standard FORTRAN, conversion.

*Nature of problem*
FORTRAN programs to be used at more than one installation are best written in ANS FORTRAN IV. Most statements are easily written in standard FORTRAN, but literal expressions require the counting of characters, and most programmers prefer to enclose literals between standard characters (apostrophes, asterisks, etc.), as allowed by many compilers. The present program converts FORMAT and DATA statements containing such literals to standard form. For example, '0TITLE.' becomes 7H0TITLE.

The standard DATA statement requires as many variables to be initialized as there are constants
DIMENSION VEC(3)
DATA VEC(1), VEC(2), VEC(3)/1.0, 2.0, 3.0/ (1)
while most compilers allow arrays to be initialized as follows:

DATA VEC/1.0, 2.0, 3.0/ (2)

or

DATA (VEC(I), I = 1, 3)/1.0, 2.0, 3.0/ (3)

The present program expands most statements of types (2) and (3) to the standard form (1). Punch code conversion can also be carried out, although less efficiently than by non-FORTRAN utility programs.

*Restrictions on the complexity of the problem*
Incorrect FORTRAN may give unpredictable results. DATA statements involving arrays with two or more subscripts, or containing two or more arrays separated by commas, are not processed. Expansion of large arrays is not recommended [DATA (VECTOR (I), I = 1, 1000)/1000*1.0/ would require some 150 cards]. Card columns 73–80 are ignored.

*Typical running time*
Compilation: 17 sec. Running time for example provided: 7 sec (IBM 360/65).

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* Present address: Cavendish Laboratory, University of Cambridge, Cambridge, UK.

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# A FLEXIBLE, ALL-PURPOSE CURVE-FITTING PROGRAM

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*Akron, Ohio 44325, USA*

Received 6 April 1976

## PROGRAM SUMMARY

*Title of program*: UNIFIT2

*Catalogue number*: ABMR

*Computer*: IBM 370/158; *Installation*: The University of Akron, Akron, Ohio, USA

*Operating system*: OS/VS2

*Programming language used*: FORTRAN IV (G)

*High speed storage required*: ⩾ 13 000 words (55 kbt)

*Number of bits in a word*: 32

*Overlay structure*: None

*Number of tapes required*: None

*Other peripherals used*: Card reader, line printer, (Calcomp incremental plotter, optional)

*Number of cards in combined program and test deck*: 1092

*Keywords*: Curve fitting, least-squares, non-linear, general purpose, variable metric minimization, theoretical models, parameter optimization, chi-square analysis, plotting.

*Nature of the physical problem*
The program fits theoretical models of arbitrary form (up to 20 parameters) to experimental data ($x$, $y$, $\Delta y$), calculates chi-square, and plots data, error bars, and fit.

*Method of solution*
A non-linear metric minimzation technique [1] is used to minimize $\chi^2$ for the spectral data, optimizing its parameters. The gradient of $\chi^2$ is calculated by a finite-difference method.

*Restrictions on program complexity*
Present dimensions limit each case to 100 data points and the model to 20 parameters; these limits may be changed by redimensioning and altering certain check statements. Arbitrarily many fit types may be accommodated without recompiling; the program performs successive fits of various types per run.

*Typical running time*
On the IBM 370/158 at The University of Akron, compilation takes about 11 CPU sec, while a typical 3–5 parameter fit to 40 points takes 3–6 sec, of which over half is spent generating the line printer plot and the Calcomp plot.

*Unusual features of the program*
The program is intended to give general fitting capabilities both for routine production work and special cases. To facilitate this,

(1) for each compilation the program may be set to fit any of several model types, for each of which the parameters may vary in number but must be the first several, the remainder serving as fixed constants,

(2) the data may be transformed before the fit; fit type and transformation may be elicited and coordinated by a code supplied with each case,

(3) the fit procedure requires estimates for each model parameter, accepts their uncertainty to speed convergence, outputs a code for the success of the fit, the uncertainty in the optimized parameters, and $\chi^2$ per degree of freedom.

*References*

[1] W.C. Davidon, U.S. Atomic Energy Commission R & D Report ANL-5990 (Rev.) Appendix (1959).

Computer Physics Communications 11 (1976) 221–236
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# COMPUTING A LAPLACIAN FIELD COMPONENT FROM BOUNDARY OBSERVATIONS ONLY

M.J. O'CONNELL
*Rutherford Laboratory, Chilton, Didcot, Oxfordshire, OX11 OQX, UK*

Received 20 November 1975

## PROGRAM SUMMARY

*Title of program:* MAGNETSUITE

*Catalogue number:* ABCM

*Computer:* IBM 360/195

*Installation:* Rutherford Laboratory

*Operating system:* IBM OS/HASP

*Programming language used:* FORTRAN

*High speed store required:* 40 kwords

*No. of bits in a word:* 32

*Overlay structure:* none

*No. of magnetic tapes required:* 1 for input in normal use

*Other peripherals used:* card reader, line printer, disk files or tapes

*Number of cards in combined program and test deck:* 3050

*Keywords:* Nuclear, experimental analysis, magnet, electrostatics, Laplace, potential, field component, boundary observation.

*Nature of physical problem*
Many physics experiments require a knowledge of magnetic field component at a grid of points within the aperture of a magnet. These are to be computed from evenly spaced observations of magnetic field made on the boundary of a hypothetical rectangular box surrounding the volume being considered.

*Method of solution*
The magnetic field component in vacuum is fully determined by its boundary values, by Maxwell's equations. Consequently it has zero laplacian and has its largest absolute value on the boundary. If it is modelled by a function which itself has a zero laplacian then the errors of representation are largest at the boundary. If these errors are acceptable, the computed values at internal points are even more so. The mathematical model is a sum of products of trigometrical and hyperbolic functions [1].

*Restrictions on the complexity of the problem*
The periodicity of the trigonometrical functions precludes extrapolation beyond the confines of the box. This is not a handicap in practice.

*Typical running time*
30 sec on IBM 360/195

*Unusual features of program*
The program suite comprises a preliminary program to read data, an analysis program to generate coefficients from the observations and a synthesis program to evaluate the field from the coefficients. To simplify changing the system from one application to another there are also two editing programs which set array dimensions and other data in the analysis and synthesis programs.

*Reference*
[1] H. Wind, Nucl. Inst. Methods 84 (1970) 117.

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# A NEW VERSION OF A PROGRAM CALCULATING THE STATIC INTERACTION POTENTIAL BETWEEN AN ELECTRON AND A DIATOMIC MOLECULE

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*Department of Applied Mathematics and Theoretical Physics,*
*The Queen's University of Belfast, Belfast, N. Ireland*

Received 19 January 1976

## PROGRAM SUMMARY

*Title of program*: OCEP W.F. and STATIC POTENTIAL

*Catalogue number*: ACWO

*Computer*: ICL 1906A; *Installation*: Atlas Computer Laboratory, Chilton, Didcot, Oxon, UK

*Operating system*: GEORGE 4

*Program language used*: FORTRAN IV

*High speed storage required*: 187K words

*No. of bits in a word*: 24

*Overlay structure*: None

*Number of magnetic tapes required*: 3 (disc files optional)

*Other peripherals used*: Card reader, card punch, line printer

*Number of cards in combined program and test deck*: 2113

*Reference to other published version of this program: Catalogue number*: ACQW; *Title*: STATIC INTERACTION POTENTIAL; *Ref. in CPC*: 2 (1971) 261

*Keywords*: Quantum chemistry, molecule, wavefunction, single-centre expansion, static potential, dipole moment, quadrupole moment, multipolar expansions, scattering.

*Nature of the physical problem*
This program calculates in one-centre, expansion (OCE) form the wavefunction for a diatomic molecule and also the multipolar expansion of its static interaction with a point charge. It corrects some errors contained in a previous version of this program [1] and provides both potential and wavefunction in a form suitable for use in a program to calculate electromolecule scattering [2].

*Method of solution*
The original two-centre wavefunction is assumed to be given by a single-determinantal (closed-shell) representation from an LCAO–MO–SCF calculation. Each of the occupied molecular orbitals (MO's) is described by an expansion over Slater-type functions (STO's) centred on either of the two nuclei of the molecule. The atomic orbitals are then expanded in Legendre polynomials around the centre of mass and the resulting single particle wavefunctions, once orthnormalized, are used to calculate the static potential.

*Restrictions on the complexity of the program*
The maximum number of basis set functions is 50, for a maximum total number of 10 MO's. The once-centre expansion of the wavefunction can be carried out up to 21 terms and the potential multipolar expansion up to 26 terms. These limits can be extended by altering the dimensions of the arrays.

*Typical running time*
To evaluate a set of MO at 1 value of $r$ takes about 0.5 sec on an IBM 30/75 machine. Similarly to evaluate a set of static potentials at one radial value $r$ takes about 0.5 sec.

*References*
[1] F.H.M. Faisal and A.L.V. Tench, Comput. Phys. Commun. 2 (1971) 261.
[2] N. Chandra, Comput. Phys. Commun. 5 (1973) 417.

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* SRC Senior Visiting Fellow. Permanent address: Istituto di Chimica Fisica dell'Università, Pisa, Italy.

Computer Physics Communications 11 (1976) 249–256
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# QUASI-BOUND STATE WAVEFUNCTIONS

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*Nuclear Structure Research Laboratory*[*], *University of Rochester, Rochester, New York 14627, USA*

Received 15 March 1976

## PROGRAM SUMMARY

*Title of program*: QUASI-BOUND STATE WAVEFUNCTIONS

*Catalogue number*: ABMQ

*Computer*: IBM 360/65; *Installation*: University of Rochester

*Operating system*: OS MVT Release 21.8

*Program language used*: FORTRAN

*High speed store required*: 175K (WATFIV compiler)

*No. of bits in a word*: 64 (double precision)

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*Number of cards in combined program and test deck*: 628

*Keywords*: Nuclear, wave function, quasi-bound, unbound, Schrödingers equation, resonant state, reaction, Woods–Saxon.

*Nature of the physical problems*
A program has been written which calculates the solution to the time independent Schrödinger equation for particles trapped by a Coulomb barrier but whose energy is greater than zero.

*Method of solution*
For fixed Woods–Saxon radius and diffuseness, the depth of the nuclear potential is iteratively found starting from a radius where the total potential energy exceeds the particle energy. Using this nuclear potential the quasi-bound wavefunction is generated from the boundary conditions at $r = \infty$ of $G(r)/r$ where $G(r)$ is the irregular Coulomb wavefunction

*Restriction on the complexity of the problem*
The program is dimensioned for a maximum of 400 mesh points and a maximum angular momentum of 10. Both these limits are easily increased if desired.

*Typical running time*
For the test case ($^{212}$Po = $^{208}$Pb + $\alpha$), 7 sec using the WATFIV compiler – this includes compilation time.

*Unusual features of the program*
Because the solution is exactly on resonance no searching on the phase shift is required. Therefore this technique works even if the resonance widths are extremely narrow ($10^{-10}$ eV for example).

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[*] Supported by the National Science Foundation.

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# PROGRAM FOR OPTIMAL COMPUTATION OF EPR SPIN-HAMILTONIAN PARAMETERS FOR IONS IN TETRAGONAL SYMMETRY

A. Sabba STEFĂNESCU
*Institute for Atomic Physics, Bucharest, Romania*

Received 18 December 1974, revised manuscript received 24 February 1976

## PROGRAM SUMMARY

*Title of program*: EPR SPIN HAMITONIAN PARAMETERS

*Catalogue number*: ACKI

*Computer*: IBM 370/168; *Installation*: Kernforschungszentrum, Karlsruhe

*Operating system*: OS

*Programming language used*: FORTRAN IV

*High speed storage required*: 14 kwords

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1147

*Keywords*: Solid-state, EPR spin-hamiltonian parameters, tetragonal environment, least squares fit, magnetic field, paramagnetic ion, fourth order perturbation

*Nature of the physical problem*
The program computes the EPR spin-hamiltonian parameters for the paramangetic ions in a tetragonal environment and an external magnetic field $H$. Its purpose is to optimize the computation of these spin-hamiltonian parameters with respect to the experimental errors. It can be used also for paramagnetic ions in cubic environment or in the absence of any of the parameters $D, A, B, a, F$. The general form of such a spin-hamiltonian with respect to the crystal axes is:

$$\mathcal{H}_{\mathrm{s}} = \beta[g_{\parallel} H_z S_z + g_{\perp}(H_x S_x + H_y S_y)] + \tfrac{1}{3} D O_2^0$$
$$+ \tfrac{1}{120}(a + \tfrac{2}{3}F) O_4^0 + \tfrac{5}{120} a O_4^4 + A S_z I_z + B(S_y I_y + S_x I_x).$$

*Method of solution*
Performing a fourth-order perturbation expansion for the above spin-hamiltonian in the cases when the applied magnetic field is parallel and perpendicular, respectively, with respect to the axis of highest symmetry, one obtains a set of nonlinear equations for the spin-hamiltonian parameters.

In the case when the number of available equations is greater than the number of parameters, a least squares minimization by an iterative procedure is carried out.

The external magnetic field $H$ was assumed to be sufficiently large to make the electronic Zeeman term dominant with respect to any other terms in the hamiltonian.

*Restriction on the complexity of the problem*
The expressions used for the transition fields are valid only for hamiltonians with tetragonal or cubic symmetry and for a dominant Zeeman term. The nuclear and the quadrupole terms are neglected.

*Typical running time*
The time required for the test run of $Mn^{2+}$ in $NH_4Cl$ is 7.55 sec on a IBM 370/168 computer, of which 6.72 sec are needed for compiling.

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# RECURSIVE EVALUATION OF 3*j* AND 6*j* COEFFICIENTS *

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and

R.G. GORDON
*Harvard University, Department of Chemistry,
Cambridge, Massachusetts 02138, USA*

Received 23 February 1976

## PROGRAM SUMMARY

*Title of program*: J1-RECURSION OF 3J-COEFFICIENTS

*Catalogue number*: ACWQ

*Computer*: UNIVAC 1108; *Installation*: Gesellschaft für wissenschaftliche Datenverarbeitung, Göttingen, Fed. Rep. Germany.

*Operating system*: EXEC 8

*Program language used*: FORTRAN 4

*High speed storage required*: 8958 words

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, lineprinter (for test)

*No. of cards in combined program and test deck:* 405

*Keywords*: General purpose, molecular, rotation group, recoupling coefficient, 3*j*, Clebsch–Gordan, Wigner, angular momentum, recursion.

*Nature of physical problem*
Subroutine REC3JJ generates 3*j* coefficients

$$f(j_1) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

for all allowed $j_1$ ($j_2, j_3, m_1, m_2, m_3$ held fixed) from the exact solution of a recursion equation. The algorithm is more efficient and accurate than those based on explicit expressions, particularly in the commonly arising case in which a complete set of 3*j* coefficients is needed. The algorithm is numerically stable for large quantum numbers which occur in problems of molecular dynamics.

*Methods of solution*
To guarantee numerical stability the recursion equation which relates 3*j* coefficients $f(j_1)$ with contiguous $j_1$ values $j_1-1$, $j_1, j_1+1$ is solved in the direction of increasing $f(j_1)$ from both ends of the allowed $j_1$ domain, $j_{1\,\min}$ and $j_{1\,\max}$. The linear recursion equation reduces to two terms at $j_{1\,\min}$ and $j_{1\,\max}$ and thus can be started at both ends with arbitrary initial values $f(j_{1\,\min})$ and $f(j_{1\,\max})$, respectively. At an intermediate $j_1$ forward and backward recursions are matched which leaves all $f(j_1)$ off by a constant factor. This factor is determined from the unitary property of 3*j* coefficients and Wigner's phase convention.

*Typical running time*
0.4 msec per 3*j* coefficient for $j_{1\,\max}-j_{1\,\min} > 20$, somewhat longer for smaller $j_1$ domains.

*Unusual features of the program*
Large quantum number 3*j* coefficients $f(j_1)$ may vary over many orders of magnitude over their $j_1$ domain. The program prevents underflow and overflow for which purpose the smallest and largest number representable on the computer, TINY and HUGE, respectively, have to be defined. In the recursion process the relative magnitudes of contiguous 3*j* coefficients $f(j_1)$ are being evaluated exactly, however. The program sets later on all 3*j* coefficients which are smaller than TINY to zero.

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* Supported by the National Science Foundation.

## PROGRAM SUMMARY

*Title of program*: M2-RECURSION OF 3J-COEFFICIENTS

*Catalogue number*: ACWR

*Computer*: UNIVAC 1108; *Installation*: Gesellschaft für wissenschaftliche Datenverarbeitung, Göttingen, Fed. Rep. Germany.

*Operating system*: EXEC 8

*Program language used*: FORTRAN 4

*High speed storage required*: 8879 words

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, lineprinter (for test)

*No. of cards in combined program and test deck*: 392

*Keywords*: General purpose, molecular, rotation group, recoupling coefficient, 3*j*, Clebsch–Gordan, Wigner, angular momentum, recursion.

*Nature of physical problem*
Subroutine REC3JM generates 3*j* coefficients

$$g(m_2) = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_1-m_2 \end{pmatrix}$$

for all allowed $m_2$ ($j_1, j_2, j_3, m_1$ held fixed) from the exact solution of an recursion equation. The algorithm is more efficient and accurate than those based an explicit expressions, particularly, in the commonly arising case in which a complete set of 3*j* coefficients is needed. The algorithm is numerically stable for large quantum numbers which occur in problems of molecular dynamics.

*Methods of solution*
To guarantee numerical stability the recursion equation which relates 3*j* coefficients $g(m_2)$ with contiguous $m_2$ values $m_2-1, m_2, m_2+1$ is solved in the direction of increasing $g(m_2)$ from both ends of the allowed $m_2$ domain, $m_{2\,\mathrm{min}}$ and $m_{2\,\mathrm{max}}$. The linear recursion equation reduces to two terms at $m_{2\,\mathrm{min}}$ and $m_{2\,\mathrm{max}}$ and thus can be started at both ends with arbitrary initial values $g(m_{2\,\mathrm{min}})$ and $g(m_{2\,\mathrm{max}})$, respectively. At an intermediate $m_2$ forward and backward recursion are matched which leaves all $g(m_2)$ off by a constant factor. This factor is determined from the unitary property of 3*j* coefficients and Wigner's phase convention.

*Typical running time*
0.3 msec per 3*j* coefficient for $m_{2\,\mathrm{max}}-m_{2\,\mathrm{min}} > 20$, somewhat longer for smaller $m_2$ domains.

*Unusual features of the program*
Large quantum number 3*j* coefficients $g(m_2)$ may vary over many orders of magnitude over their $m_2$ domain. The program prevents underflow and overflow for which purpose the smallest and largest number representable on the computer, TINY and HUGE, respectively, have to be defined. In the recursion process the relative magnitude of contiguous 3*j* coefficients $g(m_2)$ are being evaluated exactly, however. The program sets later on all 3*j* coefficients which are smaller than TINY to zero.

## PROGRAM SUMMARY

*Title of program*: J1-RECURSION OF 6J-COEFFICIENTS

*Catalogue number*: ACWS

*Computer*: UNIVAC 1108; *Installation*: Gesellschaft für wissenschaftliche Datenverarbeitung, Göttungen, Fed. Rep. Germany.

*Operating system*: EXEC 8

*Programming language used*: FORTRAN 4

*High speed storage required*: 9178 words

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, lineprinter (for tests)

*No. of cards in combined program and test deck*: 431

*Keywords:* General purpose, molecular, rotation group, recoupling coefficient, 6*j*, Racah, Wigner, angular momentum, recursion.

*Nature of physical problem*
Subroutine REC6J generates 6*j* coefficients

$$h(j_1) = \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}$$

for all allowed $j_1$ ($j_2, j_3, l_1, l_2, l_3$ held fixed) from the exact solution of a recursion equation. The algorithm is more efficient and accurate then those based on explicit expressions, particularly in the commonly arising case in which a complete set of 6*j* coefficients is needed. The algorithm is numerically stable for large quantum numbers which occur in problems of molecular dynamics.

*Methods of solution*
To guarantee numerical stability the recursion equation which relates 6*j* coefficients $h(j_1)$ with contiguous $j_1$ values $j_1 - 1, j_1, j_1 + 1$ is solved in the direction of increasing $h(j_1)$ from both ends of the allowed $j_1$ domain, $j_{1\,\mathrm{min}}$ and $j_{1\,\mathrm{max}}$. The linear recursion equation reduces to two terms at $j_{1\,\mathrm{min}}$ and $j_{1\,\mathrm{max}}$ and thus can be started at both ends with arbitrary initial values $h(j_{1\,\mathrm{min}})$ and $h(j_{1\,\mathrm{max}})$, respectively. At an intermediate $j_1$ forward and backward recursions are matched which leaves all $f(j_1)$ off by a constant factor. This factor is determined from the unitary property of 6*j* coefficients and Wigner's phase convention.

*Typical running time*
0.5 msec per 6*j* coefficient for $j_{1\,\mathrm{max}} - j_{1\,\mathrm{min}} > 20$, somewhat longer for smaller $j_1$ domains.

*Unusual features of the program*
Large quantum number 6*j* coefficients $h(j_1)$ may vary over many orders of magnitude over their $j_1$ domain. The program prevents underflow and overflow for which purpose the smallest and largest number representable on the computer, TINY and HUGE, respectively, have to be defined. In the recursion process the relative magnitudes of contiguous 6*j* coefficients $h(j_1)$ are being evaluated exactly, however. The program sets later on all 6*j* coefficients which are smaller than TINY to zero.

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# NONLINEAR COMPUTATION OF ANISOTROPIC ELASTIC FIELDS ABOUT STRAIGHT EDGE DISLOCATIONS

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Received 15 November 1975

## PROGRAM SUMMARY

*Title of program*: NONLIN

*Catalogue number*: ACKK

*Computer*: UNIVAC 1108; *Installation*: HRZ, Universität Ffm

*Operating system*: EXEC 8, 31.244

*Programming language used*: FORTRAN V

*High speed storage required*: 12 863 words

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 493

*Keywords*: Solid state, displacement, edge dislocation, elastic field, nonlinear theory, volume dilatation

*Nature of physical problem*
This program enables the user to compute the elastic boundary conditions of straight edge dislocations using a procedure derived by Seeger et al. [1] on the basis of nonlinear anisotropic elastic theory.
The result may be used to compute exactly the ionic (atomic) configuration within the dislocation core by using semi-discrete techniques.

*Method of solution*
The final formula for the nonlinear anisotropic elastic field is obtained starting from Airy's stress function. Differentiating twice gives the stresses wherefrom the strain components may be determined with the help of the 'generalized' Hooke's law. Integrating the strains finally gives the displacements.
Complex variables and constants are used to simplify difficulties arising from the mathematical complexity of the problem.

*Typical running time*
Running time for the test program is only a few seconds (about 20 sec).

*References*
[1] A. Seeger, C. Teodosiu and P. Petrasch, Phys. Stat. Solidi (b) 67 (1975) 207.

Computer Physics Communications 11 (1976) 287–297
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# IDENTIFICATION OF NUCLEAR REACTIONS REGISTERED IN IONOGRAPHIC DETECTORS

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and

C. JACQUOT
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Received 27 February 1976

## PROGRAM SUMMARY

*Title of program*: JOTOV

*Catalogue number*: ABKF

*Installation*: DCT 2000 UNIVAC Terminal, Universidad Autónoma de Barcelona

*Operating system*: EXEC 8

*Programming language used*: FORTRAN IV

*High speed storage required*: 24 Kw.

*Number of bits in a word*: 36

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, disc

*Number of cards in combined program and test deck*: 5278

*Keywords*: Nuclear, reaction, ionographic detector, experimental analysis, minimization, chi-square probability, intermediate energy, range-energy relation

*Nature of physical problem*
A nuclear reaction appears in a ionographic detector as an interaction star whose geometry can be accurately measured. Identity and energy of the incoming beam are known but the identity of the target and emergent prongs are not. Once a target has been assumed and a charge and mass number hypothesis (Z,A) has been made for each prong, the complete kinematics of the reaction can be established. All possible hyphtheses are examined under the requirements of conservation of momentum and total energy.

*Method of solution*
The chi-square function is minimized by the method of Lagrange multipliers, the conservation of momentum and energy giving the four constraints. This leads to a system of non-linear equations which are solved by an iterative procedure. Convergence of parameters and conservation values is tested during the resolution.

*Typical running time*
Typical CPU times for identification of one event in nuclear emulsion are:

| Beam | Possible targets | Number of prongs | Time (sec) |
|---|---|---|---|
| Alpha | C,N,O | 4 | 20 |
| Alpha | C,N,O | 5 | 45 |
| Alpha | C,N,O | 6 | 150 |
| Proton | C,N,O | 4 | 4 |
| Proton | C,N,O | 5 | 18 |
| Proton | C,N,O | 6 | 80 |
| Proton | C,N,O | 7 | 145 |

These times represent an average over a great number of events.

Computer Physics Communications 11 (1976) 325–330
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# SUBROUTINE FOR CALCULATION OF MATRIX PADÉ APPROXIMANTS

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*Rehovot, Israel*

Received 20 May 1976

## PROGRAM SUMMARY

*Title of program*: PADE APPROXIMANTS

*Catalogue number*: ACWV

*Computer*: IBM 370/165; *Installation*: Weizmann Institute of Science, Israel

*Operating system*: OS360

*Program language used*: FORTRAN IV

*High speed storage required*: 63000 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 686

*Keywords*: General purpose, Padé approximant, perturbation series, expansion coefficients.

*Nature of physical problem*
This computer program contains subroutines which calculate any desired Padé approximant. Given the appropriate number of coefficients in the perturbation expansion of a matrix-valued function of any given dimension, the program computes the approximant at a given point $x$.

*Method of calculation*
The calculation is carried out using a closed formula obtained in ref. [1] and completely proved in ref. [2].

*Restrictions on the complexity of the problem*
Calculations are done in double-precision mode (each number occupies two 32-bit words in memory). All the quantities calculated are kept in the active area. If matrices of large dimensions are to be used or approximants of high order calculated, the program could be easily modified to keep most of the information on tape or disk to reduce memory use.

*Typical running time*
Running time depends roughly on the square of the order of the matrices involved and on the square of the order of the approximant requested. To give an order of magnitude for the running time we mention that calculating the [6,5] Padé approximant for a three by three-dimensional problem needed 0.90 sec on an IBM 370/165. The test program enclosed needed 4.63 sec for calculating 66 Padé approximants ranging from [1,1] to [11,7] Padé approximant.

*References*
[1] H.M. Hofmann, Y. Starkand and M.W. Kirson, Perturbation theory and Padé approximants in realistic large-matrix models of the nuclear effective interaction, Nuclear Phys. A 266 (1976) 138.
[2] Y. Starkand, Weizmann Institute preprint.

Computer Physics Communications 11 (1976) 331–337
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# A SIMPLE FORTRAN PROGRAM TO INTERPRET CUBIC X-RAY POWDER DIFFRACTION DATA

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Received 1 July 1976

## PROGRAM SUMMARY

*Title of program*: XRAY2

*Catalogue number*: ABMT

*Computer*: IBM 370/158;

*Installation*: The University of Akron, Akron, Ohio, USA

*Operating system*: OS/MVT, OS/VS2

*Programming language used*: FORTRAN IV (G)

*High speed store required*: 8700 words (35 kbt)

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: None

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 618

*Keywords*: Crystallography, X-ray, diffraction, powder method, Debye–Scherrer, indexing, cubic lattice, orthorhombic, tetragonal, lattice parameter fit.

*Nature of physical problem*
Powder X-ray diffraction data can be tested for the presence and approximate amount of cubic, tetragonal, or orthorhombic lattices whose dimensions are known approximately. For cubic types, a careful determination of the lattice parameter is made.

*Method of solution*
The Bragg equation with given parameters is inverted to give primitive plane spacings, which are then associated with the nearest (if acceptable) observed lines by indices and order. For cubic types, a Taylor–Sinclair extrapolation of the lattice parameter is made, based on the identified lines.

*Restrictions on program complexity*
The present limit of 50 observed lines is easily removed by redimensioning and altering one loop parameter.

*Typical running time*
On the IBM 370/158, the program compiles (G level) in about 3 CPU sec. A typical case with 15 lines, a limit on reflection indices of six, and two hypotheses, takes about 1 sec CPU time.

*Unusual features of the program*
The program is intended as an aid in identifying powder diffraction patterns, and to make precision measurements of cubic lattice parameters.

(1) Line positions are accepted either as angles $\theta$ or as cm readings on film; in the latter case, the $\theta = 0$ position (and film shrinkage) may be found by the program and
(2) several hypothetical structures per spectrum may be tested for; line intensities are not used in the identification, but only to estimate relative identified intensity.

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# COMPUTATION OF THE ANISOTROPIC CUBIC ELASTIC GREEN'S TENSOR FUNCTION AND THE ELASTIC ENERGY COEFFICIENTS OF POINT DEFECTS IN CRYSTALS

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*und Institut für Theoretische und Angewandte Physik der Universität Stuttgart, Fed. Rep. Germany*

Received 5 January 1976

## PROGRAM SUMMARY

*Title of program*: ANISCO

*Catalogue number*: ACKL

*Computer*: Telefunken TR 440; *Installation*: Institut für Informatik, Universität Stuttgart, Herdweg 51

*Operating system*: BS 3

*Programming language used*: ALGOL 60

*High speed storage required*: 10 000 words

*No. of bits in a word*: 48

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1278

*Keywords*: Solid state, elasticity, point defect, elastic energy, volume change, Green's function, Kroener's formula, infinite medium, cubic symmetry.

*Nature of physical problem*
The elastic properties of a medium can be expressed by the elastic fundamental integral (elastic Green's tensor function for the infinite medium). It can be calculated exactly only for isotropic and hexagonal symmetry, for all others (e.g. cubic) approximations must be used.

*Method of solution*
Kroener gave an expansion of Green's function in spherical harmonics, which has the advantage of being differentiable, so that the physically important first [1] and second derivatives can be calculated. Our program calculates the expansion coefficients of Green's function and its first and second derivatives; with them the coefficients of the elastic energy and the volume change of a point defect were obtained.

*Restrictions on the complexity of the problem*
The expansion in spherical harmonics is valid for all crystal structures, but our program is restricted to cubic symmetry.

*Typical running time*
The running time depends on the degree of anisotropy of the medium and on the accuracy of the results. With a relative accuracy of $10^{-3}$ the computing time of the test run for Cu was 156 seconds.

*Reference*

[1] E. Mann, R. v. Jan and A. Seeger, Phys. Stat. Sol. 1 (1961) 17.

Computer Physics Communications 11 (1976) 353–362
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# ONE-DIMENSIONAL WAVE PACKET SOLUTIONS OF TIME-DEPENDENT FRICTIONAL OR OPTICAL POTENTIAL SCHRÖDINGER EQUATIONS

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Received 18 May 1976

## PROGRAM SUMMARY

*Title of program*: FRICTION

*Catalogue number*: ACWT

*Computers and installations*: IBM 360/91-370/145 at IPP Garching, IBM 370/165 at GSI Darmstadt

*Operating system*: HASP

*Program language used*: FORTRAN

*High speed storage required*: 140 K bytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 546

*Keywords*: Quantum mechanics, Schrödinger equation, friction, optical potential, atomic, nuclear physics, scattering

*Nature of physical problem*
Quantum mechanical treatment of classical equation of motion $m\ddot{x} + \gamma m\dot{x} + \mathrm{d}V(x)/\mathrm{d}x = 0$ (incl. $\gamma = 0$), by time dependent nonlinear Schrödinger equations or solution of arbitrary (including optical) hamiltonians.

*Method of solution*
Finite difference method

*Restrictions on the complexity of the program*
One-dimensional motion.

*Typical running time*
Depending on problem 0.5...5 min.

*Unusual features of the program*
Double precision complex arithmetic (IBM type COMPLEX*16) is used. It should be replaced by single precision complex arithmetic if run on a computer with more than approximately ten digits of accuracy.

Computer Physics Communications 11 (1976) 363–368
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# NON-RELATIVISTIC FORM FACTOR PROGRAM FOR COMPTON SCATTERING OF GAMMA RAYS BY BOUND ELECTRONS

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*II. Physikalisches Institut der Universität, D-3400 Goettingen, Fed. Rep. Germany*

Received 22 June 1976

## PROGRAM SUMMARY

*Title of program*: COMPTON CROSS SECTIONS

*Catalogue number*: ACWW

*Computer*: UNIVAC 1108; *Installation*: GWDG Goettingen

*Operating system*: EXEC 8

*Programming language used*: FORTRAN IV

*High speed storage required*: 12 000 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, printer

*No. of cards in combined program and test deck*: 761

*Keywords*: atomic, gamma ray scattering, Compton scattering, form factor, cross-section profile, spectroscopy.

*Nature of physical problem*

The program Compton cross sections performs the calculation of the cross-section profile for Compton scattering of gamma rays by the electrons of a complete subshell of an atom on the basis of non-relativistic hydrogen-like one-electron wave functions [1].

*Method of solution*

Closed-form expressions for the cross-section profile derived in ref. [1] are used.

*Restrictions on the complexity of the problem*

For energies of the scattered gamma rays near the free-electron value convergence may be too slow.

*Typical running time*

On the Univac 1108 computer less than a few minutes are required in most cases.

*Unusual features of the program*

Different effective atomic numbers may be used for the scattering electron in the initial bound state and the final continuum state, respectively.

*Reference*

[1] M. Schumacher, F. Smend and I. Borchert, J. Phys. B: Atom. Molec. Phys. 8 (1975) 1428.

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# BOLTZ: A CODE TO SOLVE THE TRANSPORT EQUATION FOR ELECTRON DISTRIBUTIONS AND THEN CALCULATE TRANSPORT COEFFICIENTS AND VIBRATIONAL EXCITATION RATES IN GASES WITH APPLIED FIELDS

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*Centre for Computer Studies, The University, Leeds, UK*

and

A.R. DAVIES
*Department of Computing, Royal Holloway College, Englefield Green, Surrey, UK*

Received 27 May 1976

## PROGRAM SUMMARY

*Title of program*: BOLTZ

*Catalogue number*: ACWX

*Computer*: ICL 1906A; *Installation*: University of Leeds

*Operating system*: George 4

*Programming language used*: FORTRAN

*High Speed Store Required*: 200 K words

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter

*No. of cards in a combined program and test deck*: 2857

*Keywords*: Boltzmann equation, electron distribution, Transport coefficients, vibrational excitation rates, laser physics, plasma physics.

*Nature of physical problem*
BOLTZ is a set of two programs which calculates the electron distribution, transport coefficients, and electron vibrational excitation rates in a gas mixture with an applied electric field. With the test deck provided, BOLTZ calculates the excitation rates needed for TLASER [1] – a laser kinetics code for $CO_2$:$N_2$:He lasers. Given the necessary cross-section data BOLTZ will calculate the electron distribution, etc. for any gas mixture.

*Method of solution*
The program solves the time-independent Boltzmann equation for the electron energy distribution function in a gas mixture. Following Rockwood [2] the Boltzmann equation is written in terms of the electron number density. By partitioning the electron energy axis into $K$ cells the time independent Boltzmann equation is converted to a set of $K$ simultaneous linear equations. The equivalent matrix equation is first solved ignoring the effects of superelastic collisions, in which case the matrix is upper Hessenberg. The solution of the matrix equation then proceeds rapidly by back-substitution. The vibrational excitation rates and transport coefficients are then obtained as the appropriate weighted integrals over the electron number density distribution. The program then solves the matrix equation taking into account the effect of superelastic collisions. The matrix is then a full matrix and the solution for the electron distribution is first obtained for a coarse mesh by converting the matrix to upper triangular form by column pivoting and solving by back substitution. The solution is interpolated to a fine mesh and is used as the initial guess to solve the matrix equation by Gauss–Seidel iteration.

*Restrictions on the complexity of the problem*
Up to nine gases may be included. The value of the applied field has an upper limit set by the amount of store available for the matrix elements.

*References*

[1] A.R. Davies, K. Smith and R.M. Thomson, Comput. Phys. Commun. 10 (1975) 117.
[2] S.D. Rockwood, Phys. Rev. A8 (1973) 2348.

Computer Physics Communications 11 (1976) 385–395
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# CALCULATION OF THE FORM OF AN EQUILIBRIUM POLOIDAL MAGNETIC FIELD CONTAINED IN A POLYTROPIC STAR

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and

M.J. MIKETINAC*
*Mathematics Research Center, University of Wisconsin-Madison, Madison, WI 53706, USA*

Received 5 November 1976

## PROGRAM SUMMARY

*Title of program*: POLOID

*Catalogue number*: AAAI

| *Computer*: | *Installation*: |
|---|---|
| UNIVAC 1106 | Computer Centre, University of Cape Town |

*Operating system*: EXEC 8

*Programming language used*: FORTRAN

*High speed storage required*: 68K

*No. of bits in a word*: 36

*Overlay structure*: No

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 2350

*Catalogue number*: AAAE; Title: TOROID; Ref in CPC: 7 (1974) 410

*Keywords*: Astrophysics, polytropic star, equilibrium configuration, poloidal magnetic field

*Nature of physical problem*
This program is designed to integrate the exact equations which determine the distribution of the density of a self-gravitating, axisymmetric polytrope of infinite conductivity containing a poloidal magnetic field [1]. In addition, other properties of an equilibrium configuration such as mass, volume and radius are calculated. The program can also provide at very small extra cost the rates of change of the density with respect to changes of the polytropic index $n$ and the parameter $\lambda$ which characterizes the poloidal magnetic field.

*Method of solution*
Mathematically, the problem can be formulated as a boundary value problem for three coupled equations, two of which are second order, non-linear, two-dimensional partial differential equations. The solution is obtained numerically by an adaptation of the Stoeckly's finite difference-finite expansion method [2]; in fact, the present program is a major modification of the program TOROID published in ref. [2].

*Restrictions on the complexity of the problem*
As in ref. [2], the numerical scheme developed in the program is valid for all polytropes whose polytropic index $n$ is greater than or equal to one. The other parameter of the theory, $\lambda$, is unrestricted, i.e. the program permits the study of stars whose magnetic energy is a "sizeable" percentage of their gravitational energy. Also, the program, with minor modifications, could be used for calculating equilibrium configurations of (a) (uniformly or non-uniformly) rotating polytropes pervaded by poloidal magnetic fields or (b) (rotating) polytropes containing poloidal magnetic fields or a more general type than the one considered in ref. [1]. However, the greatest use of the present program is expected to arise in attempts to construct equilibrium configurations of polytropes containing mixed poloidal toroidal magnetic fields.

*Typical running time*
The time required for the test run is 8 min 28 sec on a UNIVAC 1106 computer, of which 5.06 sec is taken in compiling.

*References*
[1] M.J. Miketinac, Astrophys. Space Sci. 35 (1975) 349.
[2] M.J. Miketinac, Comput. Phys. Commun. 7 (1974) 410.

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* On leave from the University of Cape Town.

Computer Physics Communications 11 (1976) 397–405
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# A PROGRAM TO CALCULATE ANGULAR MOMENTUM COEFFICIENTS IN RELATIVISTIC ATOMIC STRUCTURE – REVISED VERSION

I.P. GRANT

*Department of Theoretical Chemistry, University of Oxford,
1 South Parks Road, Oxford, UK*

Received 19 February 1976

## PROGRAM SUMMARY

*Title of program*: MCP75

*Catalogue number*: ACWE

*Computer*: IBM 360/195;
*Installation*: Rutherford Laboratory, Chilton, Berks, UK

*Operating system*: OS/360, Hasp.

*Programming language used*: FORTRAN IV

*High speed storage required*: 102 K bytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 2465

*CPC Libary subprograms used*:

| *Catalogue number* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAGD | NJSYM | 1 (1970) 241<br>2 (1971) 173 |
| AAGD0002 | ADAPT TO INTEGER ARITHMETIC | 5 (1973) 161 |
| ACRI | CFPJJ-CFP IN JJ-COUPLING | 4 (1972) 377 |

*Reference to other published version of this program*:
Catalogue number: ACRJ; Title: MCP; Ref. in CPC: 5 (1973) 263

*Keywords*: Atomic, Configuration interaction, Racah, fractional parentage, recoupling coefficients, Slater integrals, complex atoms, relativistic, Dirac equation, wave function, *jj*-coupling, theoretical methods.

*Nature of physical problem*
Many calculations of atomic properties require the use of a multiconfiguration description of the wave function. The present program MCP75, constituting an adaptation of the original version of MCP [1], to use double-precision floating-point arithmetic on IBM machines together with corrections and modifications, expresses the matrix elements of the inter-electronic Coulomb repulsion between *jj*-coupled configuration wave functions constructed using Dirac central field single electron orbitals in terms of a linear combination of relativistic Slater integrals. The coefficients of this combination are computed by the program in a form suitable for use in multiconfiguration Dirac–Fock programs such as those of Desclaux [2] or Grant et al. [3] and in similar applications.

*Method of solution*
Configurational states are defined by the number of electrons in each occupied shell, the quantum numbers (nja) or (nk) for each such shell, and angular momenta specifying the coupling scheme. Matrix elements between such states can be written in the form

$$\sum_{k} \sum_{\alpha\beta\gamma\delta} C_k(\alpha\beta\gamma\delta)\, R^k_c(\alpha\beta\gamma\delta)\,;$$

the coefficients $C_k(\alpha\beta\gamma\delta)$ calculated by this program are expressed as products of recoupling coefficients and coefficients of fractional parentage. For details, see ref. [1].

*Restrictions on the complexity of the problem*
The program assumes that both configurations are formed from the same orthonormal set of basis orbitals. The number of electrons in a shell having $j \geqslant 9/2$ is restricted to be not greater than 2 by the available cfp routines. The present version allows up to 10 orbitals and 30 configurational states together with 100 coefficients but these numbers can be changed by the user. The user should ensure that the CPC Library Subprograms AAGD, ACRI have been converted to use double precision floating point arithmetic before running with MCP75.

*References*

[1] I.P. Grant, Comput. Phys. Commun. 5 (1973) 263.
[2] J.P. Desclaux, Comput. Phys. Commun. 9 (1975) 31.
[3] I.P. Grant, D.F. Mayers and N.C. Pyper, to be published.

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Computer Physics Communications 11 (1976) 407
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# ERRATUM NOTICE

*Title of manuscript*: Multistate molecular treatment of atomic collisions in the impact parameter approximation. I. Integration of coupled equations and calculation of transition amplitudes for the straight line case.

*Authors*: C. Gaussorgues, R.D. Piacentini and A. Salin

*Reference*: Computer Physics Communications 10 (1975) 223

*Title of program*: PAMPA

*Catalogue number*: ACWJ

Computer Physics Communications 12 (1976) 147–162
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# FOURGEN: A FAST FOURIER TRANSFORM PROGRAM GENERATOR

J.A. MARUHN
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Received 27 July 1976

## PROGRAM SUMMARY

*Title of program*: FOURGEN

*Catalogue number*: ABUO

*Computer*: IBM 360/91 and 360/195; *Installation*: Oak Ridge National Laboratory

*Operating system*: OS/360

*Programming language used*: PL/1 (ref. [1]) and ASA FORTRAN

*High speed storage required*: 270 kBytes

*No. of bits in a byte*: 8

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, sequential output device (card punch, disk, or tape)

*No. of cards in combined program and test deck*: 600

*Keywords*: General purpose, fast Fourier transform, Fourier, analysis, synthesis, sine analysis, cosine analysis, harmonic, generator.

*Nature of the problem*
FOURGEN generates specialized fast-Fourier-analysis codes based on the Hockney general-purpose code FOOR67 [2]. Each code is performing one of the four transform types (sine analysis and synthesis, cosine analysis and synthesis, periodic analysis, and periodic synthesis) on a real vector of fixed length.

*Method of solution*
FOURGEN is basically a PL/1 translation of FOUR67, with eh exception that those parts of the code that actually operate on the input data are not executed but punched out as a complete Fortran subroutine. This eliminates essentially all program overhead.

*Restrictions on the complexity of the program*
FOURGEN is able to generate subroutines for all types of transforms mentioned above and all dimensions $N = 2^{\mathrm{IQ}} + 1$ with IQ $\geqslant 3$. However, for IQ $\geqslant 7$ the size of the generated subroutines increases so fast that they may be useful only under very special circumstances.

*Typical running times*
On the 360/91 the generation of a subroutine with IQ $< 7$ always took less than 1 sec. Performance characteristics for the generated programs are discussed in detail in the long write-up. In general they are a factor of 2–4 faster than FOUR67.

*References*
[1] OS PL/1 checkout and Optimizing Compilers: Language Reference Manual (IBM Order No. GC33-0009-3).
[2] J.P. Christiansen and R.W. Hockey, Comput. Phys. Commun. 2 (1971) 127.

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* Research sponsored by the US Energy Research and Development Administration under contract with Union Carbide Corporation.

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Computer Physics Communications 12 (1976) 163–171
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# SEQUENTIAL RANDOM INTEGER GENERATOR *

C.T.K. KUO , T.W. CADMAN and R.J. ARSENAULT
*University of Maryland, College Park, Maryland 20742, USA*

Received 4 October 1976

## PROGRAM SUMMARY

*Title of program*: SRNG

*Catalogue number*: ACIE

*Computer*: UNIVAC 1108; *Installation*: University of Maryland, College Park, Maryland, U.S.A.

*Operating system*: UNIVAC 1108 EXEC

*Program language used*: FORTRAN

*High speed storage required*: 17000 words.

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: Optional

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 106

*Keywords*: General, random integer, generator, solid solution strengthening.

*Nature of physical problem*
An algorithm to generate a subset of random integers from a larger set of integers has been developed to minimize both the computing time and the memory space. The algorithm deals with the whole array at the same time, generates a subset of random integers for a given percentage of the range, and the generated subset of random integers is obtained as sequentially increasing numbers. Such random integers are used to specify the positions of randomly dispersed impurity atoms or solute atoms in many computer simulation experiments. A specific case is that of solid solution strengthening.

*Method of solution*
In order to produce a large subset of sequentially increasing, non-repeating random integers from a larger set of integers, each integer of the larger set is represented by a bit of a computer word. On the UNIVAC 1108, 35 bits can be used to represent 35 integers of the larger set, the remaining sign bit is used to indicate a particular word location.

Two groups of random numbers are generated, which are uniformly distributed in the interval 0 to 1. Group 1 is used to choose the computer word, and Group 2 is used to choose the bit within the computer word.

*Restrictions on the complexity of the problem*
The number of integers from which the random subset can be chosen is limited by the size of the computational cell. The cell is limited by the computer storage capacity.

*Typical running time*
To select a sequential subset of $2.8 \times 10^4$ non-repeating random integers from a larger set of $2.8 \times 10^6$ integers requires ~15 minutes of UNIVAC 1108 memory time. However, changing the total number of integers does not result in a linear change in the computer time. The time required to select a subset of $2.8 \times 10^3$ sequential non-repeating random integers from a larger set of $2.8 \times 10^5$ integers is ~3 seconds.

*Unusual features of the program*
Two unusual features of this program are the use of one's compliment representation of minus zero and bit manipulation capability in the UNIVAC 1108 computer.

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* This work was supported by a NASA Grant No. NSG-3001, and the Computer Science Center of the University of Maryland.

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# ALGORITHMS FOR THE KAC AND RENYI TESTS

J.M.F. CHAMAYOU

*CERN – Data Handling Division, Geneva, Switzerland*

Received 28 September 1976

## PROGRAM SUMMARY

*Title of program*: RENYIF, RENYIT, TESKAC

*Catalogue number*: ACXB

*Computer*: CDC 7600; *Installation*: CERN, Geneva

*Operating system*: CDC Scope

*Programming language*: FORTRAN IV

*High speed store required*: 10155 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program test deck*: 600

*Keywords*: General, statistics, goodness of fit tests, asymptotic Renyi distribution, Renyi test, Random size sample test, KAC test.

*Nature of physical problem*
Given a sample (with fixed size for the Renyi test and random size for the Kac test) of independent observations of a random variable having an unknown continuous distribution function $G(x)$. The hypothesis $G(x) = F(x)$ for a given $F(x)$ is tested using the empirical distribution function.

*Method of solution*
The observations are ranked in increasing order to calculate the empirical distribution function. The maximum of the absolute difference between $F(x)$ and the empirical distribution function is computed and the test of the hypothesis is performed using the asymptotic Renyi distribution.

*Restriction on the complexity of the problem*
The size of the sample must be large enough to allow a valid use of the asymptotic Renyi distribution.

*Running time*
Depends on the size of the sample and on the algorithm used to rank the observations in increasing order.

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# COULOMB COEFFICIENTS FOR COMPLEX IONIC CRYSTALS

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*Carnegie Laboratory of Physics, The University, Dundee, Scotland*

Received 27 July 1976

## PROGRAM SUMMARY

*Title of program*: KCOULI

*Catalogue number*: ACWY

*Computer*: ICL System 4/75, ICL 2980 system B

*Installation*: Edinburgh Regional Computing Centre

*Operating system*: Edinburgh Multi-Access System (EMAS)

*Programming language*: ALGOL 60

*High speed store required*: 4000 words (object code)

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 925

*Keywords*: Solid state, lattice dynamics, external modes, coulomb coefficients, complex ionic crystals

*Nature of physical problem*

The program evaluates Coulomb coefficients for complex ionic crystals using the equations given by Venkataraman and Sahni [1] modified to take account of the work of Scheringer [2]. These equations are a generalization of the ones given by Kellermann [3].

*Method of solution*

The efficient evaluation of several convergent complex three-dimensional sums is central to the problem of obtaining the coefficients. The terms which control the convergence of the sums along the $x$, $y$ and $z$ axes have been identified, together with limiting values for them.

In the program preliminary calculations along the axes are made to find the indices at which the limiting values are reached. These indices are used as limits when calculating the sums in full.

*Restrictions on the complexity of the problem*

The symmetry of the crystal must be orthorhombic (P, F or I, but not C) or higher. There must only be two ions or ionic groups per primitive unit cell.

*References*

[1] G. Venkataraman and V.C. Sahni, Rev. Mod. Phys. 42 (1970) 409.
[2] C. Scheringer, Acta Cryst. A30 (1974) 359.
[3] E.W. Kellermann, Phil. Trans. Roy. Soc. A238 (1940) 513.

Computer Physics Communications 12 (1976) 199–203
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# MULTISTATE MOLECULAR TREATMENT OF ATOMIC COLLISIONS IN THE IMPACT PARAMETER APPROXIMATION. III – INTEGRATION OF COUPLED EQUATIONS AND CALCULATION OF TRANSITION AMPLITUDES FOR COULOMB TRAJECTORIES

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*Université de Bordeaux I,*
*33405 Talence,*
*France*

Received 29 June 1976

## PROGRAM SUMMARY

*Title of program*: TANGO

*Catalogue number*: ACWU

*Computer*: IRIS 80

*Installation*: Centre de Calcul Interuniversitaire, Bordeaux, France

*Operating system*: SIRIS 8

*Program language used*: FORTRAN

*High speed storage required*: 100K words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 904

*Keywords*: Atomic, molecular, collisions, impact-parameter method, semi-classical, Coulomb trajectories, coupled equations

*Nature of the physical problem*
Multistate molecular treatment of atomic collisions in the impact parameter approximation [1]. Calculation of the transition amplitudes for Coulomb classical trajectories.

*Method of solution*
The coupled first-order differential equations are integrated by the method of Bulirsch and Stoer. The integrals over energy differences are integrated by Simpson's rule.

*Restriction on the complexity of the problem*
Coulomb trajectories only. Typical running time: running time for the test run: 2.83 min on the IRIS 80.

*References*
[1] C. Gaussorgues, R.D. Piacentini and A. Salin, Comput. Phys. Commun. 10 (1975) 223.

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* Equipe de recherche CNRS No. 137.

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Computer Physics Communications 12 (1976) 205–212
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# COLLRAD: A CODE FOR CALCULATING THE QUASI-STEADY STATE POPULATION DENSITIES OF EXCITED STATES OF HYDROGEN-LIKE IONS

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Received 6 October 1976

## PROGRAM SUMMARY

*Title of program*: COLLRAD

*Catalogue number*: AAID

*Computer*: UNIVAC 1108 and 1100/42; *Installation*: Australian National University, Canberra

*Operating system*: EXEC-8

*Programming language used*: FORTRAN

*High speed store required*: 14620 words

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used:* Line printer, card reader

*No. of cards in combined program and test deck*: 1360

*Keywords*: Collisional, radiative, recombination, ionization, hydrogen-like, population density, plasma, spectroscopy, atomic, astrophysics.

*Nature of physical problem*

The evaluation of the population densities of the lower quantum states of a plasma ion, in general, involves the simultaneous solution of the rate equations (one for each quantum state) containing the rates of the various collisional and radiative processes which populate and de-populate each quantum state. We consider the time independent case where quasi-steady state equilibrium is established.

*Method of solution*

COLLRAD calculates quantum state densities for hydrogen-like ions using the collisional-radiative model of Bates et al. [1] and McWhirter and Hearn [2]. Coefficients giving the population densities of the excited states, and the rate of change of the ground state density are calculated for input electron density and temperature by solving a set of simultaneous linear equations.

*Restrictions on the complexity of the problem*

Densities are calculated for excited quantum states in quasi-steady state equilibrium.

*Typical running time*

For execution 1.7 sec on the ANU UNIVAC 1100/42.

*Unusual features of the program*

COLLRAD is written in standard FORTRAN, except for the use of the NAMELIST facility.

*References*

[1] D.R. Bates, A.E. Kingston and R.W.P. McWhirter, Proc. Roy. Soc. A267 (1962) 297.
[2] R.W.P. McWhirter and A.G. Hearn, Proc. Phys. Soc. 82 (1963) 641.

Computer Physics Communications 12 (1976) 213–230
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# GLOWCODE: A ONE-DIMENSIONAL CODE FOR THE SIMULATION OF PLASMA AFTERGLOWS

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and

M.C. SEXTON
*University College, Cork, Ireland*

Received 7 October 1976

## PROGRAM SUMMARY

*Title of program*: GLOWCODE

*Catalogue number*: ABUP

*Computer*: ICL System 4; *Installation*: Culham Laboratory

*Operating system*: Multijob

*Programming languages used*: FORTRAN

*High speed store required*: 24000 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other preipherals used*: line printer

*No. of cards in combined program and test deck*: 2489

*CPC library subprograms used*: Catalogue no: ABUF; *Title*: OLYMPUS; *Ref. in CPC*: 7 (1974) 245.

*Keywords*:
Plasma physics, afterglow, ionization, radiative, recombination, diffusion, implicit, lagrangian

*Nature of physical problem*
GLOWCODE is a one-dimensional cylindrical code which simulates the decay of a hydrogen plasma in which the dominant loss mechanism is three body collisional–radiative recombination. In addition the processes of ionization, radiation, diffusion, heat conduction and equipartition are described. Optically thin conditions are assumed; the limiting case of complete opacity can be studied with the appropriate choice of atomic coefficients [1].

*Method of solution*
The afterglow is described by the variables $n_e$, $n_i$, $n_a$, $T_e$, $T_i$, $T_a$ which represent the electron density, the ion density, the atom density, electron temperature, ion temperature and atom temperature, respectively. The cylindrical volume is divided into a system of concentric shells and the computation proceeds by solving the various collisional–radiative processes taking place within each shell, and by computing the energy transfer across each shell to its neighbour. At each stage of the calculation pressure balance is re-established by adjusting the cylindrical shells, changing the plasma parameters adiabatically, until the pressure gradient is zero across the plasma radius. Implicit numerical schemes are used for the solution of the conduction and diffusion equations so that there is no stability restriction on the time step for the spatially dependent equations.

*Restrictions on the complexity of the problem*
The number of cyclindrical mesh points can be varied up to a maximum of 41 in the existing program. *Ad hoc* changes can be made to the code using the EXPERT facility provided by the OLYMPUS package [2].

*Typical running time*
The execution time depends on the number of mesh points required and on the print out frequency. On the ICL 1905 at Oxford Polytechnic a typical run using 21 mesh points with a print out every 100 steps takes around 1100 sec to compute 1000 time-steps. i.e. 0.05 sec/mesh point/time step approximately. The ICL 4/70 at Culham Laboratory takes approximately one-fifth of this time.

*Unusual features of the program*
GLOWCODE uses the NAMELIST facility which is not a STANDARD FORTRAN feature. The modular structure and the use of the OLYMPUS package provide the prospective user with a highly adaptable program for the investigation of hydrogen afterglows.

Under certain conditions the calculation could possibly fail if highly non-equilibrium pressure situations arise. This is because in the establishment of pressure equilibrium an iterative implicit numerical technique is applied which may not converge if large departures from pressure equilibrium develop. A reduction in the time step should remedy this effect.

*References*

[1] J.W. Long and A.A. Newton, Xth Int. Conf. on Ionization Phen. in Gases, Oxford (1971) 1.1.3.7.
[2] J.P. Christiansen and K.V. Roberts, Comput. Phys. Commun. 7 (1974) 245.

Computer Physics Communications 12 (1976) 231–236
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# CALCULATION OF THE ENERGY RESPONSE OF A SPECTROMETER

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*UER Scientifiques, 29283 Brest Cedex, France*

Received 3 August 1976

## PROGRAM SUMMARY

*Title of program*: AFER

*Catalogue number*: ACXA

*Computer*: IBM 1130; *Installation*: University of Bretagne Occidentale, Brest, France

*Operating system*: V2M11

*Programming language used*: FORTRAN IV

*High speed store required*: 8168 words

*Number of bits per word*: 16

*Overlay structure:* None

*Number of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, disk, incremental plotter (optional)

*Number of cards in the combined program and test deck*: 880

*Keywords*: Plasma physics, radiative transfer, spectral line width, quantitative spectroscopy, convolution integral.

*Nature of the physical problem*
This program computes the convolution integral of an idealized spectrograph (or spectrometer) apparatus function with a Voigt line profile (lorentzian and gaussian shaped line). On this basis one could evaluate the validity to derive the total integrated intensity of an emission (or absorption) line from the peak value of the recorded signal (irradiance for a spectrograph, radiant power for a spectrometer).

*Method of solution*
The various functions and convolution integrals, i.e. source function (convolution of a gaussian line shape with a Lorentz line) and apparatus function (convolution of entrance slit function, grating function, exit slit function) are evaluated by Fourier transform. These direct and inverse Fourier transforms are computed numerically using the discrete Fourier transform with a method derived from the Cooley–Tukey algorithm [1].

*Restriction of the complexity of the problem*
For our physical problem, according to the computer used for each function calculated, the number of samples is limited to 512 ($2^9$). The final response is given with 256 ($\frac{1}{2}2^9$) points.

With a trivial change the program can compute with another resolution for the total bandpass, or with other forms of the various functions.

*Typical running rime*
The test run takes about 140 sec on the IBM 1130.

*Reference*

[1] J.W. Cooley and J.W. Tukey, Math. Comput. 19 (1965) 297.

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Computer Physics Communications 12 (1976) 237–257
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# PIPIT: A MOMENTUM SPACE OPTICAL POTENTIAL CODE FOR PIONS *

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*Department of Physics, Carnegie-Mellon University, Pittsburgh, Pennsylvania 15213, USA*

Frank TABAKIN
*Department of Physics, University of Pittsburgh, Pittsburgh, Pennsylvania 15260, USA*

Received 2 September 1976

## PROGRAM SUMMARY

*Title of program*: PIPIT

*Catalogue number*: ABIH

*Computer*: UNIVAC 1108; *Installation*: Computer Center, Carnegie-Mellon University, Pittsburgh, Pa. 15213 USA. Program also runs on CDC 6600 and 7600; DEC PDP-10

*Operating system*: UNIVAC EXEC II

*Program language*: FORTRAN IV

*High speed storage required*: $35216_{10}$

*No. of bits in a word*: 36

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1683

*CPC library subprograms used*: cat. no. ABCJ; *title*: PIRK, ref. in CPC: 8 (1974) 130.

*Keywords:* Nuclear, pion, elastic scattering, angular distribution, cross section, optical potential, momentum space, Lippmann–Schwinger equation.

*Method of solution*
Angular distributions for the elastic scattering of pions are generated by summing a partial wave series. The elastic $T$-matrix elements for each partial wave are obtained by solving a relativistic Lippmann–Schwinger equation in momentum space using a matrix inversion technique. Basically the Coulomb interaction is included exactly using the method of Vincent and Phatak [1]. The $\pi$N amplitude is obtained from phase shift information on-shell and incorporates a separable off-shell form factor to ensure a physically reasonable off-shell extrapolation. The $\pi$N interaction is of finite range and a kinematic transformation procedure is used to express the $\pi$N amplitude in the $\pi$ nucleus frame.

*Restrictions on the complexity of the program*
A maximum of 30 partial waves can be used in the present version of the program to calculate the cross section. The Lippmann–Schwinger equation is presently solved for each partial wave by inverting a 34 × 34 supermatrix. At very high energies, larger dimensions may be required. The present version of the code uses a separable non-local $\pi$N potential of finite range; other types of non-localities, or non-separable potentials, may be of physical interest.

*Typical running time*
This depends on the number of partial waves and the size of the supermatrix. The test case requires 60 sec on the UNIVAC 1108 (10 partial waves, 34 × 34 supermatrix).

*Reference*
[1] C.M. Vincent and S.C. Phatak, Phys. Rev. C10 (1974) 391.

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* Work supported by the Unites States ERDA [Contract AT(11-1)3244] and the NSF.

Computer Physics Communications 12 (1976) 277–292
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# A PROGRAM FOR CALCULATING THE OBSERVABLES FOR SINGLE-PARTICLE-INCLUSIVE PRODUCTION REACTIONS

K.J.M. MORIARTY and J.H. TABOR
*Department of Mathematics, Royal Holloway College, Englefield Green, Surrey TW20 OEX, UK*

Received 11 August 1976

## PROGRAM SUMMARY

*Title of program*: ONCPLT

*Catalogue number*: AAUR

*Computer*: CDC 6600, CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: CDC SCOPE

*Programming language used*: FORTRAN IV

*High speed store required*: 25 K words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, printer, Calcomp plotter with Calcomp compatible software

*No. of cards in combined program and test deck*: 4020

*Cat. No.*: AAUN; *Title*: APLOT; *Ref. in CPC*: 9 (1975) 85

*Keywords*: nuclear, high energy, single-particle-inclusive cross section, $s$-channel helicity states, spin density matrix, effective trajectories, $\chi^2$-minimization, graph plotting

*Nature of the physical problem*
This program is concerned with the phenomenological analysis and the display via both the printer and graph plotter of high-energy single-particle-inclusive production reaction observables.

*Method of solution*
The program can be run under either the fixed $t$ or the fixed $M^2$ modes when calculating differential cross sections with that for fixed $t$ being integrated over the $t$-bin by 8-point Gaussian quadrature. Total cross sections can be calculated using repeated 48-point Gaussian quadrature. In addition, effective trajectories and density matrix elements can be calculated. The results of all these types of calculation can be plotted with the inclusion of the graph plotting package APLOT [1]. The program is compatible with MINUIT [2] and this combination has been used to perform minimization [3].

*Restrictions on the complexity of the program*
The number of data points considered cannot exceed 500 in general. In the case where density matrix data or effective trajectory data is to be read in the number of data points cannot exceed 100. This is purely a dimensional requirement and can be altered. If density matrices are to be calculated the final detected particle must have spin less than 5/2.

*Typical running time*
The test run took 72.2 sec (of which 32.7 sec was compilation time). A recent minimization calculation [3] in which the program was used, 400 passes minimizing three parameters on 28 data points took 184 sec.

*References*

[1] J. Anderson, K.J.M. Moriarty and R.C. Beckwith, Comput. Phys. Commun. 9 (1975) 85.
[2] F. James and M. Roos, Comput. Phys. Commun. 10 (1975) 343.
[3] K.J.M. Moriarty and J.H. Tabor, Nuovo Cim. Lett. 16 (1976) 362.

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Computer Physics Communication 12 (1976) 293–303
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# EXACT FINITE-RANGE MICROSCOPIC CALCULATIONS FOR HEAVY-ION INDUCED TWO-NUCLEON TRANSFER REACTIONS *

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and

K.S. LOW
*Jabatan Fizik, Universiti Malaya , Kuala Lumpur, Malaysia*

Received 25 October 1976

## PROGRAM SUMMARY

*Title of program*: SATTNT-FOR-EFR-MICRO-DWBA

*Catalogue number*: ABMU

*Computer*: CDC 6600; *Installation*: University of Texas Computation Center

*Operating system*: UT2D

*Programming language used*: FORTRAN IV

*High speed store required*: 45248 words

*Number of bits per word*: 60

*Overlay structure*: yes

*Number of magnetic tapes required*: 5

*Other peripherals used*: Card reader, line printer, punch

*Number of cards in combined program and test deck*: 3158

*Keywords*: Nuclear, heavy ions, direct nuclear reactions, exact-finite-range microscopic DWBA, form factor, stripping, pickup, cross section, elastic scattering, Schroedinger equation, EFR-MICRO-DWBA.

*Nature of physical problem*
The program SATTNT calculates the form factor for two-nucleon transfer reactions. The approach adopted in this program is the exact-finite-range microscopic theory [1]. The created form factor is to be used, for instance, in the MARS-1 program [2] to calculate the DWBA cross sections.

*Method of solution*
The radial part of the wave functions of the bound nucleons are expanded in terms of oscillator functions and then Moshinsky transformed by using a program developed by Feng and Tamura [3]. To evaluate the kernels of EFR form factors, one-dimensional integrals are carried out by Gaussian quadrature, introducing a specific technique [2] so as to minimize the number of quadrature points. Throughout the program interpolation and other techniques [2] are used so that an EFR calculation can be performed reasonably quickly.

*Restrictions on the complexity of the program*
Restrictions on the size of the calculation come about mostly from the number allowed for the pairs $(L_1, L_2)$, where $L_1$ and $L_2$ are orbital angular momenta of the center-of-mass motion of the two transferred nucleons, respectively, in the donor and acceptor nuclei. However, only a very small number of pairs actually contribute to the reaction and the storage presently assigned will meet the needs of most practical calculations.

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* Work supported in part by the US Energy Research and Development Administration.

*References*

[1] D.H. Feng, T. Udagawa and T. Tamura, Nucl. Phys., A274 (1976) 262.

[2] T. Tamura and K.S. Low, Comput. Phys. Commun. 8 (1974) 349.

[3] D.H. Feng and T. Tamura, Comput. Phys. Commun. 10 (1975) 87.

Computer Physics Communications 12 (1976) 305–321
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# A PROGRAM FOR THE CALCULATION OF THE POSITIONS OF X-RAY POWDER REFLECTIONS

I.F. FERGUSON, R.S. FOX and T.E. HUGHES
*Materials Science Group, UKAEA, Springfields, Preston, UK*

Received 6 July 1976

## PROGRAM SUMMARY

*Title of program*: FIREBIRD 2

*Catalogue number*: AAQD

*Computer*: ICL 4-72; *Installation*: UKAEA, Risley, UK

*Operating system*: J 1700

*Programming language used*: FORTRAN IV

*High speed storage required*: 291 half kilobytes

*Number of bits in a half byte*: 4

*Overlay structure*: None

*Number of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer

*Number of cards in combined program and test deck*: 4072

*Keywords*: Crystallography, X-ray, powder diffraction, Bragg reflection positions, interplanar angles, indexing, space groups, Laue groups.

*Nature of the physical problem*
The program, FIREBIRD, calculates the position of Bragg reflections in X-ray powder diffraction for all crystal systems and Laue groups for a given set of crystal lattice parameters. The general conditions which limit the possible reflections from any space group are allowed for. The program can vary the lattice parameters systematically and since provision is made for comparing the position of calculated and observed Bragg angles FIREBIRD can, in principle, aid in the assignment of Miller indices to any (single phase) X-ray powder diffraction pattern. The program can also be used to generate interplanar angles, crystallographic densities and can produce lists of Miller indices in a form suitable for transcription as input to the program FIREFLY [1].

*Method of solution*
All the calculations described are carried out using standard X-ray powder diffraction formulae; where necessary, X-ray reflections not allowed by the general space group symmetry are suppressed.

*Restrictions on the complexity of the problem*
The program is restricted to the output of data which relate to 1000 permitted Bragg reflections. In the case of the triclinic and rhombohedral crystal systems FIREBIRD only considers the first 10 000 computed Miller indices before output is commenced. No more than 17 different wave-lengths can be handled in any example.

*Typical running time*
1 min for a typical example

*Unusual features of the program*
Some non-standard FORTRAN statements are used including RETURN $n$ to provide alternate return points from subroutine

*References*

[1] I.F. Ferguson and J.E. Kirwan, Comput. Phys. Commun. 5 (1973) 328;
I.F. Ferguson, Comput. Phys. Commun. 10 (1975) 42.

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Computer Physics Communications 12 (1976) 323–334
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# PULSAMP: A PROGRAM TO PREDICT THE AMPLIFICATION OF NANOSECOND $CO_2$ LASER LIGHT PULSES

S.A. ROBERTS and Kenneth SMITH
*Centre for Computer Studies, University of Leeds, Leeds, UK*

Received 24 June 1976

## PROGRAM SUMMARY

*Title of program*: PULSAMP

*Catalogue number*: AC × C

*Computer*: ICL 1906A; *Installation*: University of Leeds, Computing Centre

*Operating System*: George 4

*Programming language used*: FORTRAN

*High speed store used*: 65 K words

*No. of bits in a word*: 48

*Overlay structure*: None

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 1246

*Keywords*: Laser amplifier, rotational coupling, $CO_2$, extracted energy

*Nature of the physical problem*
PULSAMP is a program which predicts the behaviour of a light pulse of duration ~1 nsec as it propagates through a gain medium. Singleline or multiline/multiband operation may be simulated. The laser medium consists of a pre-pumped $CO_2$, $N_2$, He mixture.

*Method of solution*
Initially the laser medium is described by the population number densities, $N^{10^\circ 0}$, $N^{00^\circ 1}$ and $N^{02^\circ 0}$, of the 10°0, 00°1 and 02°0 vibrational levels of $CO_2$. These population number densities are assumed initially to be constant within the laser cavity. Partial differential equations, which take into account the effects of stimulated transitions from the 00°1 vibrational level to the 10°0 and/or 02°0 vibrational level(s), as well as coupling among the rotational sublevels within each vibrational level, describe the propagation of a given input light pulse through the gain medium, and the time history of the population inversions. We follow Armandillo and Spalding [1] in solving these equations by employing Simpson's rule swept over a two-dimensional (space–time) grid.

*Restrictions on the complexity of the problem*
The model used neglects the effect of coherent propagation of the pulse (see, for example, ref. [2], Section 13.3) and is therefore not valid for describing the propagation of pulses of duration less than the dipole dephasing time [3]. Also neglected are the effects of all V–V and V–T transitions, so the pulse duration is further restricted to be less than the fastest V–V transition times.

For the input pulse profile with respect to time, either an analytic shape is assumed, or experimental values may be read. The code is written to generate two analytic pulse shapes; rectangular or gaussian.

*Typical running time*
For the sample output given at the end of the paper the running time is 280 sec on the ICL 1906A. Running time is dependent upon duration of the input pulse, number of transitions in the input pulse, and the laser cavity length.

*References*

[1] E. Armandillo and I.J. Spalding, J. Phys. D, 8 (1975) 2123.
[2] M. Sargent III, M.O. Scully and W.E. Lamb, Jr., Laser Physics (Addison-Wesley, Reading, Mass., 1974).
[3] R.H. Pantell and H.E. Puthoff, Fundamentals of Quantum Electronics (John Wiley and Sons, Inc., New York, 1969).

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Computer Physics Communications 12 (1976) 335–338
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# ADAPTATION OF A PROGRAM FOR DEPTH DISTRIBUTION OF ENERGY DEPOSITION BY ION BOMBARDMENT: CALCULATION OF ION LATERAL RANGES *

Irwin MANNING, Mervine ROSEN and J.E. WESTMORELAND
*Radiation Technology Division, Naval Research Laboratory, Washington, D.C. 20375, USA*

Received 4 October 1976

## ADAPTATION SUMMARY

*Title of adaptation*: Calculate Lateral Ranges

*Adaptation number*: 0001

*Reference to original program*: catalogue number: ACIB; title: E-DEP-1; ref. in CPC 7 (1974) 85.

*Authors of original program*: Irwin Manning and G.P. Mueller

*High speed store required*: 14 736 words

*No. of bits in a word*: 48

*No. of cards required to effect adaptation (including directive cards)*: 61

*Additional keywords*: Lateral range

*Purpose of the adaptation*
To calculate the lateral range of heavy ions and to extend the lowest energy considered by E-DEP-1 down to 1 keV.

*Method of solution*
Moments of the range distribution already calculated in a subroutine of E-DEP-1 are combined to obtain the lateral range.

## ERRATUM NOTICE

*Title of manuscript*: Depth distribution of energy deposition by ion bombardment.

*Authors*: Irwin Manning and G.P. Mueller

*Reference*: Comput. Phys. Commun. 7 (1974) 85

*Title of program*: E-DEP-1

*Catalogue number*: ACIB

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* This work was supported in part by the Office of Naval Research under their Contract Research Program, TASK RR 021-03-02.

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# THE BESSEL FUNCTIONS $J_0$ AND $J_1$ OF COMPLEX ARGUMENT *

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Received 23 August 1976
Revised manuscript received 26 January 1977

## PROGRAM SUMMARY

*Title of program*: BESSEL

*Catalogue number*: ACWZ

*Computer*: CDC 6600, CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: CDC SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required:* 2264 (BESSEL), 482 (CJ0), 627 (CJ1) words

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 536

*Keywords*: general purpose, atomic, molecular, nuclear, expansion, representation, eikonal, impact parameter, helicity, partial wave, Bessel functions, complex functions

*Nature of physical problem*
The Bessel function appears in a wide range of physical applications. The package Bessel contains complex function routines to calculate $J_0(z)$ and $J_1(z)$ for complex $z$. Bessel functions of higher order $n \leqslant |z|$ can be generated by resorting to recurrence relations.

*Method of solution*
The method of solution is based on analytic approximations given in [1].

*Restrictions on the complexity of the problem*
The polynomial approximations are designed for $|z| \leqslant 10$. The program will return results for $J_0(z)$ and $J_1(z)$ for all values of $|z|$ up to machine overflow. For $|z| \leqslant 10$, the maximum absolute error is less than 0.00046, whereas for $|z| > 10$, the results diverge quite rapidly from their actual values. The accuracy for $|z| \leqslant 10$ is sufficient for most physical applications, and the polynomial approximations provide a quicker calculation of Bessel functions than the use of the ascending series formula given in [1], particularly for values of $|z|$ near 10.

*Typical running time*
The test run output reproduced at the end of the Long Write Up took 0.207 sec.

*References*

[1] M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables (Dover Publications, Inc., New York, 1968).

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* Part of the Royal Holloway College Special Functions Mathematics Project.

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# A PROGRAM TO CALCULATE CORONAL EMISSION LINE STRENGTHS

P.L. DUFTON
*Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast, N. Ireland*

Received 5 November 1976

## PROGRAM SUMMARY

*Title of program*: AATWAB

*Catalogue number*: ACXE

*Computer:* ICL 1906S; *Installation*: Computer Centre, Queen's University, Belfast BT7 1NN, United Kingdom

*Operating system*: GEORGE 4

*Program language used*: FORTRAN IV

*High speed storage required*: 47K words

*No. of bits in a word*: 24, 2 words per floating point variable

*Overlay structure*: none

*Other peripherals used*: Card reader, line printer, scratch disc store

*No. of cards in combined program and test deck*: 2046

*Keywords*: Astrophysics, solar corona, emission line, excitation rate, level population, optically thin, plasma

*Nature of the physical problem*
This computer program is used to calculate the intensities of emission spectral lines from the upper solar atmosphere. The optically thin approximation is used and the validity of this assumption is checked by calculating line centre optical depths. Account may be taken of collisional transitions (by electron and proton impact) and spontaneous radiative transitions between all the selected levels of the chosen ion in calculating the intensities. The program integrates these intensities through whatever model atmosphere is selected. The calculation may be done for any position on the solar disk with the assumption of spherical symmetry for the atmosphere.

*Method of solution*
Steady-state rate equations are set up and then inverted to yield level populations for the ion under consideration. These level populations lead directly to emission line strengths for an optically thin plasma. For a model calculation this process is repeated at each depth point and the emission line strengths integrated over depth to yield total specific intensities.

*Restrictions on the complexity of the program*
Up to 50 levels can be incorporated into the model atom with each fine structure level being counted separately and up to 100 individual transitions and 10 multiplets included in the emission line strength calculations. If a depth dependent model is being considered a maximum of 101 depth points can be used.

*Typical running time*
Running time is proportional to the square of the number of levels in the model atom and to the number of depth points in the coronal model. The test run took 40 sec on the ICL 1906S.

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# RADIO RECOMBINATION LINES FROM H$^+$ REGIONS AND COLD INTERSTELLAR CLOUDS: COMPUTATION OF THE $b_n$ FACTORS

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and

M. SALEM
*Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB3 0HE, UK*

Received 26 January 1977

## PROGRAM SUMMARY

*Litle of program*: GENERAL BN PROGRAM

*Catalogue number*: ACXI

*Computer*: IBM 370/165; *Installation*: University of cambridge Computer Laboratory

*Operating system*: OS

*Programming language used*: FORTRAN IV

*High speed storage required:* 43000 words

*No. of bits in a word*: 32

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, (optional) card punch

*No. of cards in combined program and test deck*: 1291

*Keywords*: Astrophysics, radioastronomy, HII region, cold cloud, thermal source, recombination line.

*Nature of physical problem*

Emission lines produced by the recombination of hydrogen and hydrogenic ions are observed from many astronomical sources; maser amplification is frequently present. The recombination line spectrum depends upon the populations of the energy levels of the emitting species. The present program computes the ratio, $b_n$, of the population of energy level $n$ to the (known) population in thermodynamic equilibrium for given values of electron temperature and density A background radiation field may be present. The results are accurate for the range of temperatures and densities associated with cold clouds, H$^+$ regions, and planetary nebulae (10–20 000 K, $10^{-4}$–$10^{6}$ cm$^{-3}$).

*Method of solution*

The method is that described by Brocklehurst [1,2], but with the collision cross-sections of Gee et al. [3]. In statistical equilibrium, the rates of population and depopulation of each of the infinitely many energy levels must be equal. The infinite system of linear algebraic equations thus defined is truncated, and correction terms are added to compensate for the omitted levels. The resulting system is condensed to a smaller size and solved.

The equations of radiative transfer must in principle be solved simultaneously with the population equations. In practice it is usually sufficient to consider the optical depth for each line to be either zero (no absorption) or infinite (on-the-spot absorption).

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*References*

[1] M. Brocklehurst, Mon. Not. Roy. Astron. Soc. 148 (1970) 417.

[2] M. Brocklehurst, Astrophys. Lett. 14 (1973) 81.

[3] C.S. Gee, I.C. Percival, J.G. Lodge and D. Richards, Mon. Not. Roy. Astron. Soc. 175 (1976) 209.

Computer Physics Communications 13 (1977) 49–56
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# A PROGRAM FOR THE STUDY OF SHORT RANGE ORDER OF BINARY ALLOYS

G.L. BLERIS and Ch. POLATOGLOU
*2nd Laboratory of Physics, University of Thessaloniki, Greece*

Received 5 February 1976

## PROGRAM SUMMARY

*Title of program*: SROCASE

*Catalogue number*: ACKN

*Computer*: UNIVAC 1106; *Installation*: Computer Centre, Univ. of Tessaloniki

*Operating system*: EXEC8

*Programming language used*: FORTRAN IV

*High speed storage required*: 9 K

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used* : card reader, printer

*No. of cards in combined program and test deck*: 555

*Keywords*: solid state, crystal lattice, fcc, binary alloy, Cowley–Warren parameter, PVM, Newton–Raphson method, cluster, diffuse intensity profile, diffraction pattern, vacancy

*Nature of the physical problem*
The program SROCASE was developed in order to calculate the mean distribution of vacancies in an f.c.c. lattice using data related to the diffuse scattered intensity [1] in diffraction patterns and to reconstruct the patterns. Thus, from the diffraction data the Cowley–Warren s.r.o. parameters [2] are estimated and the clusters that satisfy these coefficients are obtained by the probability variation method (PVM) [3].

*Method of solution*
To determine the s.r.o. coefficients $a_i$ a Monte Carlo integration was performed over a domain $D$ defined in such a manner that at a point $x \in D$ the integrand function has a value given by the diffraction data.

The PVM requires the solution of a set of simultaneous nonlinear equations by the Newton–Raphson method. Application of this method leads to the solution of a system of linear equations by the Gauss method.

*Restrictions on the problem*
The determinant of the simultaneous linear equations must be different from zero.

*Typical running time*
The time to calculate the first 8 s.r.o. parameters and the maximum probability and to print a diffuse intensity profile is 232 sec. The for time each additional diffuse intensity profile is 84 sec.

*Unusual features of the program*
By modifying FUNCTION DOMAIN other diffuse intensity data may be reproduced.

*References*

[1] G.L. Bleris, T. Karakostas, J. Stoemenos and N.A. Economou, Phys. Status Solidi 34 (1976) 243.
[2] J.M. Cowley, Phys. Rev. 77 (1950) 669.
[3] P.C. Clapp, Phys. Rev. B, 4 (1971) 255.

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Computer Physics Communications 13 (1977) 57–62
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# MULTISTATE MOLECULAR TREATMENT OF ATOMIC COLLISIONS IN THE IMPACT PARAMETER APPROXIMATION. II – CALCULATION OF DIFFERENTIAL CROSS-SECTIONS FROM THE TRANSITION AMPLITUDES FOR THE STRAIGHT LINE CASE

R.D. PIACENTINI
*Laboratoire d'Astrophysique *, Université Bordeaux I, 33405 Talence, France and*
*Departamento de Física, Facultad de Ciencias Exactas e Ingeniería,*
*Universidad Nacional de Rosario, 2000-Rosario, Argentina*

and

A. SALIN
*Laboratoire d'Astrophysique *, Université de Bordeaux I, 33405 Talence, France*

Received 3 January 1977

## PROGRAM SUMMARY

*Title of the program*: EIKON

*Catalogue number*: ACXD

*Computer*: IRIS 80; *Installation*: Centre de Calcul Interuniversitaire, Bordeaux, France

*Operating system*: SIRIS 8

*Program language used*: FORTRAN

*High speed storage required*: 86 K words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 644

*CPC Library subprogram used (for data)*: Cat. No.: ACWJ; *Title*: PAMPA; ref. in CPC: 10 (1975) 223

*Keywords*: Atomic, molecular, collisions, impact-parameter method, semi-classical, eikonal, differential cross-sections.

*Nature of the physical problem*
Multistate molecular treatment of atomic (or molecular) collisions in the impact parameter approximation. Calculatio of eikonal differential cross-sections.

*Method of solution*
The integration over impact parameters is transformed into a partial wave expansion. The treatment of all impact parameter dependent phases is discussed in detail.

*Restriction on the complexity of the problem*: small angle scattering.

*Typical running time*: running time for the test run on the IRIS 80: 1.52 min.

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* Equipe de recherche CNRS No. 137.

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# A COMPUTER PROGRAM FOR CALCULATION OF THE CORIOLIS EFFECT IN ODD-*A* NUCLEI

R. KACZAROWSKI
*Department of Physics IA, Institute for Nuclear Research, 05–400 Świerk, Poland*

Received 9 December 1976

## PROGRAM SUMMARY

*Title of the program*: CORIOLIS

*Catalogue number*: ABQF

*Computer*: CDC CYBER 73; *Installation*: Institute for Nuclear Research, Świerk, Poland

*Operating system*: SCOPE 3.4.1

*Programming language used*: FORTRAN

*High speed storage required*: 5600 words + 9300 words for MINUIT

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 390

*CPC Library subprogram used*:

*Catalogue number*: ACWH; *Title*: MINUIT; *Ref. in CPC*: 10 (1975) 343

*Keywords*: nuclear, spectroscopy, particle–rotation coupling, Coriolis effect, fitting, experimental, energy level

*Nature of physical problem*
In recent years, many papers have been devoted to particle–rotation coupling (Coriolis effect) in nuclei, e.g. [1–4]. Dramatic perturbations due to strong Coriolis coupling are observed in the rotational bands associated with high-*j* intrinsic states (e.g. $i_{13/2}$ or $h_{9/2}$). Calculations, in which the Nilsson model [5] was extended to include Coriolis coupling [6] and pairing interaction, in many cases successfully explain the observed peculiar structure of the rotational bands. The program calculates the perturbed rotational energy levels. It is written as a subroutine for use with the MINUIT minimization program [7], which makes a least-squares fit to the experimental energy levels. The mixed amplitudes of the wave functions can be obtained for the final fit.

*Method of solution*
In order to take the Coriolis coupling into account, the energy matrix is constructed and diagonalized. The Jacobi diagonalization method is used repeatedly to solve the secular determinants for all spin values, simultaneously adjusting all the parameters until a least-squares fit to the experimental energy levels is obtained.

*Restriction on the complexity of the problem*
The current version is dimensioned for 13 interacting rotational bands based on single-particle states, a maximum spin $I = 39/2$, and 20 experimental energy levels.

*Typical running time*
The running time depends on the number of mixing bands and the number of free parameters. Therefore the required time may vary from less than one to many minutes on the CDC CYBER 73.

*References*
[1] G. Løvhøiden and I. Kanestrøm, Phys. Norv. 6, no. 1 (1972) 33.
[2] G. Løvhøiden, P.O. Tjøm and L.O. Edvardson, Nucl. Phys. A194 (1972) 463.
[3] S.A. Hjorth, A. Johnson and G. Ehrling, Nucl. Phys. A184 (1972) 113.
[4] P. Hornshøj, P. Tidemand-Petersson, R. Kaczarowski, B. Kotlińska and J. Zylicz, Nucl. Phys. A248 (1975) 406.
[5] S.G. Nilsson, C.F. Tsang, A. Sobiczewski, Z. Szymański, S. Wycech, C. Gustafson, I. Lamm, P. Möller and B. Nilsson, Nucl. Phys. A131 (1969) 1.
[6] A.K. Kerman, Mater. Fys. Medd. Dan. Vid. Selsk., no. 15 (1956) 30.
[7] F. James and M. Roos, Comput. Phys. Commun. 10 (1975) 343.

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## ERRATUM NOTICE

*Title of manuscript*: A multiconfiguration relativistic Dirac–Fock program

*Author*: J.P. Desclaux

*Reference*: Comput. Phys. Commun. 9 (1975) 31

*Title of program*: Multiconfiguration relativistic Dirac–Fock

*Catalogue number*: ACRV

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## ERRATUM NOTICE

*Title of manuscript*: Calculation of Canterburry approximants

*Authors*: P.R. Graves-Morris and D.E. Roberts

*Reference*: Comput. Phys. Commun. 10 (1975) 234

*Title of program*: FORTRAN CALCULATION OF C.A.'s

*Catalogue number*: ACWF and

*Title of program*: ALGOL CALCULATION OF C.A.'s

*Catalogue number*: ACWG

In the subroutine/procedure CANTAT there are instances when IG is undefined, namely when NX = L = 1; and when ID is undefined, namely when NY = L = 1.

Computer Physics Communication 13 (1977) 101–105
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# A PORTABLE TEXT EDITOR

Colin DAY
*Computer Centre, University College London, London, UK*

Received 1 February 1977

## PROGRAM SUMMARY

*Ttitle of program*: STRING REPLACEMENT PROGRAM

*Catalogue number*: ACXJ

| *Computer*: | *Installation*: |
|---|---|
| IBM 360/65 | University College, London |
| CDC 7600 | Univ. of London Comp. Centre |
| CDC 6400 | Imperial College, London |

*Operating system or monitor under which the program is executed*: OS MFT

*Programming language used*: FORTRAN

*High speed storage required*: c.8000 words

*No. of bits in a word*: 32

*Overlay structure*: no

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, other as required

*No. of cards in combined program and test deck*: 283

*Keywords*: general purpose, utility, editor, preprocessor, program generator

*Nature of physical problem*
A portable editor is needed for amending programs.

*Method of solution*
The String Replacement Program is a fully portable program written mostly in ANSI Basic Standard FORTRAN.

*Restrictions on the complexity of the problem*
Only character strings of the same length can be replaced.

*Typical running time*
Less than 1 sec per 1000 cards on a CDC 7600.

*Unusual features of the program*
Incorporates fully portable character manipulation.

*Reference*
[1] A.C. Day, Fortran techniques (Cambridge University Press, 1972).

Computer Physics Communications 13 (1977) 107–115
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# A FORTRAN PROGRAM TO SIMULATE QUADRUPOLE-DISTORTED NMR POWDER PATTERNS

E.D. von MEERWALL
*Physics Department, The University of Akron, Akron, Ohio 44325, USA*

Received 3 January 1977

## PROGRAM SUMMARY

*Title of program*: HEQSIM2

*Catalogue number*: ABMW

*Computer*: IBM 370/158; *Installation*: The University of Akron, Akron, Ohio 44325, USA

*Operating system*: OS/MVT; OS/VS2

*Programming language used*: FORTRAN IV (G)

*High-speed store required*: 25 000 words (101 kbt) exclusive of loader

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, Calcomp incremental plotter

*Number of cards in combined program and test deck*: 988

*Keywords:* nuclear magnetic resonance, spectrum, powder pattern, line shape, simulation, quadrupole distortion, dipolar broadening, chemical shift, absorption, dispersion, derivative

*Nature of physical problem*
The effects of a quadrupole interaction, dipolar broadening, and a chemical shift on the NMR spectrum (static) of a nucleus of arbitrary spin $1 \leqslant I \leqslant 5$ are simulated and plotted.

*Method of solution*
Perturbation results are used to produce satellite powder patterns and central transition ($m = 1/2$ to $-1/2$) in second order quadrupolar theory, and anisotropic chemical shift in first order. The Kramers–Kronig relations are used to transform absorption to dispersion mode, and gaussian or lorentzian convolution functions simulate dipolar broadening. Histographic techniques are used for the central trnasition. Inhomogeneities in the quadrupolar interaction are simulated by adding discrete component spectra.

*Restrictions on program complexity*
Within the limitations of the program, no extensions are appropriate.

*Typical running time*
On the IBM 370/158, execution per case ranges from about 15 sec for $I = 1$ or $3/2$ and low, homogeneous quadrupole interaction to over 4 min for inhomogeneous anisotropic cases of high quadrupole interaction per dipolar broadening, and dispersion mode. Compilation (FORTRAN G compiler) takes about 16 CPU sec .

*Unusual features of the program*
To maximize the utility and flexibility of the program, the following features are provided:

(1) most aspects of the simulations are self-scaling with optional enlargement factors;

(2) up to five $\nu_Q$-values per simulation provide inhomogeneity; five simulations with different $\eta$ are produced per case, with derivatives; absorption or dispersion mode may be selected; lorentzian or gaussian dipolar broadening may be of different size for central transition and satellites;

(3) full chemical shift (3 components) is simulated; shift effects should be smaller than quadrupole effects; and

(4) a plot of resonance derivative vs. field, scalable for direct comparison with experiment, is optional, and consists of the components of different asymmetry.

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# LINEAR AND NONLINEAR IDEAL MHD CODES – V103 *

H.R. HICKS and J.W. WOOTEN

*Computer Sciences Division at Oak Ridge National Laboratory, Union Carbide Corporation, Nuclear Division, Oak Ridge, TN 37830, USA*

Received 28 July 1976

## PROGRAM SUMMARY

*Title of program*: 2LDV103

*Catalogue number*: ABVQ

*Computers*: IBM 360/91; *Installation*: X-10 Computing Center, Oak Ridge National Laboratory, Oak Ridge, TN

*Operating system*: OS/360 with HASP II

*Programming language used*: PL1 with preprocessor [1]

*High speed storage required*: 224K bytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: disk (optional), line printer, card reader

*No. of cards in combined program and test deck*: 1506

*Keywords*: Plasma physics, magnetic confinement, MHD stability, operator codes, preprocessing

*Nature of physical problem*
The linearized ideal MHD equations are advanced in time. Given an unstable MHD equilibrium, the result is the largest growth rate and the corresponding eigenmode. The geometry is a rectangular cylinder with conducting walls and periodic on the ends.

*Method of solution*
An explicit leap-frog time advancement scheme is used on a cartesian grid. The finite difference scheme is space and time centered. Eventually, the fastest growing eigenmode dominates.

*Restrictions on the complexity of the system*
Only large scale instabilities can be well represented on the finite difference grid. Lower growth rates may be missed due to faster growing numerical instabilities. The user should realize that large areas of parameter space have not been tested. Although we have run many cases which we believe are valid, we make no representation that results are valid for other than the case reported here.

*Typical running times*
The run time is strongly dependent on the data. The case given in the test deck takes 2.14 min to compile, link edit, and execute on a 360/91.

*Unusual features of the program*
Heavy use is made of the IBM PL1 preprocessor [1].

*Reference*
[1] We have exclusively used the Pl/I Optimizing Compiler, Version 1 release 2.2, which is on IBM Program Product described in PL/I Checkout and Optimizing Compilers: Language Reference Manual (IBM) SC33-0009.

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* Research sponsored by ERDA under contract with Union Carbide Corporation.

## PROGRAM SUMMARY

*Title of program*: N3DV103

*Catalogue number*: ABUR

*Computers*: IBM 360/91: *Installation*: X-10 Computing Center, Oak Ridge National Laboratory, Oak Ridge, TN

*Operating system*: OS/360 with HASP II

*Programming language used*: IBM PL1 Optimizing Compiler with preprocessor [1]

*High speed storage required*: 260K bytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: disk (optional), line printer, card reader

*No. of cards in combined program and test deck*: 1497

*CPC Library subprograms used*: none

*Keywords*: Plasma physics, magnetic confinement, MHD evolution, operator codes, preprocessing, nonlinear

*Nature of physical problem*

The ideal MHD equations are advanced in time. Given an MHD configuration, the result is the evolution of that configuration. The geometry is a rectangular cylinder with conducting walls and periodic on the ends.

*Method of solution*

An explicit leap-frog time advancement scheme is used on a cartesian grid. The finite difference scheme is space and time centered.

*Restrictions on the complexity of the system*

Only large scale instabilities can be well represented on the finite difference grid. The user should realize that large areas of parameter space have not been tested. Although the authors have run many cases which we believe are valid, we make no representation that results are valid for other than the case reported here.

*Typical running times*

The run time is strongly dependent on the data. The case given in the test deck takes 22.24 min to compile, link edit, and execute on a 360/91.

*Unusual features of the program*

Heavy use is made of the IBM PL1 preprocessor [1].

*Reference*

[1] We have exclusively used the PL/I Optimizing Compiler, Version 1 release 2.2, which is on IBM Program Product described in PL/I Checkout and Optimizing Compilers: Language Reference Manual (IBM) SC33-0009.

Computer Physics Communications 13 (1977) 137–140
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## ERRATUM NOTICE

*Title of manuscript*: A program for computing level crossings and the Back Goudsmit effect

*Author*: P. Violino

*Reference*: Comput. Phys. Commun. 4 (1972) 128

*Title of program*: Back-Goudsmit

*Catalogue number*: ACRD

---

*Authors*: R.A. Eisenstein and F. Tabakin, *Title of manuscript*: PIPIT – a momentum space optical potential code for pions, *Reference*: Comput. Phys. Commun. 12 (1976) 237.

An error was corrected in the program PIPIT, resulting in changes in the test run output from that published. Test run output from the corrected deck available from the CPC Program Library as catalogue number ABIH is reproduced below. Intending users should note that this deck is complete and no other library program is required for its operation.

Computer Physics Communications 13 (1977) 167–182
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# COMPUTER SIMULATION OF CORRELATED SELF-DIFFUSION VIA RANDOMLY MIGRATING VACANCIES IN CUBIC CRYSTALS

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and

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*Institut für Theoretische und Angewandte Physik der Universität Stuttgart, 7 Stuttgart, West Germany*

Received 26 April 1977

## PROGRAM SUMMARY

*Title of program*: RANDOM VACANCY MIGRATION

*Catalog number*: ACKO

*Computer*: CDC 6600; *Installation*: University of Stuttgart

*Operating system*: Scope 3.4

*Programming language used*: FORTRAN IV

*High speed storage required*: 58 000 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No of cards in combined program and test deck*: 718

*Keywords*: solid state physics, crystal lattice, vacancy, correlated self-diffusion, random migration, fcc, bcc, simple cubic, NMR, computer simulation, Monte Carlo method, correlation factor

*Nature of physical problem*
Computer simulation of the relative jumps of atoms induced by a randomly migrating single or double vacancy [1] in a face-centered cubic, body-centered cubic, or simple cubic crystal lattice [2].

*Method of solution*
The random vacancy jumps are simulated using a procedure for the creation of a sequence of random numbers (Monte-Carlo method).

*Restrictions on the complexity of the problem*
The number of atoms the relative motions of which may be studied is limited by the lengths of the required arrays (see section 3.3 of the long write-up).

*Typical running time*
About 50 sec for the simulation of the diffusion via monovacancies in a bcc lattice. The running time is proportional to the product of the number of jumps in each encounter with the number of encounters.

*Unusual features of the program*
The program as it stands is used for NMR studies of self-diffusion (see next paper in this issue). But, with few changes it may be used for simulating very common diffusion problems, including annealing of vacancies at different kinds of sinks.

*References*

[1] A. Seeger and H. Mehrer, in: Vacancies and Interstitials in Metals, A. Seeger, D. Schumacher, W. Schilling and J. Diehl, eds. (North-Holland Publ. Co., Amsterdam, 1970) p. 1.
[2] D. Wolf, Phys. Rev. B10 (1974) 2710.

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* The basic computer program underlying this paper was developed during the author's appointment at the Max-Planck-Institut für Metallforschung, Institut für Physik, in Stuttgart, West Germany.

Computer Physics Communications 13 (1977) 183–191
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# DETERMINATION OF CORRELATION FACTOR AND NMR DIFFUSION PARAMETERS FROM THE COMPUTER-SIMULATED RANDOM MOTION OF VACANCIES IN CUBIC CRYSTALS

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Received 26 April 1977

## ADAPTATION SUMMARY

*Title of adaptations*: CORRELATION FACTOR AND NMR

*Adaptation number*: 0001

*Reference to original program*: *Catalogue number*: ACKO; *Title*: RANDOM VACANCY MIGRATION; *Ref. in CPC*: preceding paper

*Authors of original program*: D. Wolf and K. Differt

*Peripherals used*: Card reader, line printer, card punch, extended core storage ($31000_8$ words)

*No. of cards required to effect adaptation*: 169

*Keywords*: solid state physics, crystal lattice, vacancy, correlated self-diffusion, random migration, fcc, bcc, simple cubic, NMR, computer simulation, Monte Carlo method, correlation factor

*Nature of physical problem*
Combined with the program presented in the preceding paper [1], this computer program may be used for calculating
(i) the geometrical correlation factor associated with the correlated movements of individual atoms for vacancy-induced self-diffusion in cubic crystals [2], as well as
(ii) the basic quantities associated with the interpretation of NMR studies of self diffusion, such as the correlated *relative* geometrical displacements of any two atoms, and their total number of relative jumps in encounters [3] with mono- or divacancies in cubic crystals.

*Method of solution*
Simple sums over displacement probabilities of atoms, which are calculated by the program discussed in the preceding paper.

*Restriction on the complexity of the problem*
Only sc, bcc, and fcc crystal structures for monovacancy diffusion, and bcc and fcc lattice structures for self diffusion via divacancies are considered.

*Typical running time*
As an example, the test run simulates self diffusion via monovacancies in a bcc lattice. Approximately 9 sec are required for compilation and 53 sec for execution. The running time depends strongly on the values of IMAX, NLMAX and NMR (see section 3).

*Unusual features of the program*: none

*References*

[1] D. Wolf and K. Differt, Comput. Phys. Commun. (preceding paper) 13 (1977) 000.
[2] A.D. Le Claire, in: Physical Chemistry, Vol. X, H. Eyring, D. Henderson and W. Jost, eds. (Academic Press, New York and London, 1970) ch. 5.
[3] D. Wolf, Phys. Rev. B10 (1974) 2710.

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* The basic computer program underlying this paper was developed during the author's appointment at the Max-Planck-Institut für Metallforschung, Institut für Physik, In Stuttgart, West Germany.

Computer Physics Communication 13 (1977) 193–202
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# A NEW VERSION OF AAKL (THE MATRIX ELEMENTS OF SPIN–ORBIT INTERACTION) ADAPTED TO SPECTROSCOPIC NOTATION *

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Received 29 April 1977

## PROGRAM SUMMARY

*Title of the program*: SPINORBIT WEIGHTS 2

*Catalogue number*: ACXL

*Computer*: Amdahl 470 V/6; *Installation*: University of Alberta, Edmonton, Alberta, Canada

*Operating system*: MTS

*Programming language used*: FORTRAN IV

*High speed core required*: 25590 bytes

*No. of bits per byte*: 8

*Overlay structure*: none

*Other peripherals used*: card reader, line printer, card punch

*No. of magnetic tapes required*: none

*No. of cards in combined program and test deck*: 1952

### CPC library subprograms used

| *Catalogue numbers* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACQB | P SHELL C.F.P. | 1 (1969) 15 |
| ACRN | A NEW D SHELL CFP | 6 (1973) 88 |
| AAGD * | NJSYM | 1 (1970) 241<br>2 (1971) 173 |
| AAGD0001 * | ADAPT NJSYM FOR WEIGHTS | 2 (1971) 180 |
| AAGD0002 * | ADAPT TO INTEGER ARITHMETIC | 5 (1973) 161 |

*Reference to other published version of this program*: *Cat. no*: AAKL; *Title*: SPINORBIT WEIGHTS; *ref. in CPC*: 9 (1975) 102. *Keywords*: Atomic structure, fine structure, configuration interaction, complex atoms, $L-S$ coupling, spin–orbit coupling, atomic spectra.

*Nature of the physical problem*
This program is a revision of Klotz's [1] program for calculation of the matrix elements of the one-body spin–orbit interaction using multiconfigurational wave-functions. A recent correction [2] has been included in the present version.

*Purpose of the revision*
The input and output formats have been changed to a more familiar, readable and convenient spectroscopic notation. In addition, a punch option has been added to punch the results which could be directly used for energy levels calculation for various $J$-manifolds.

*Typical running time*
Time of 1.1 seconds is required for the testrun on Amdahl 470 V/6.

*Special feature*
This is a double-precision program suitable for computers with short word lengths such as the IBM S360, Amdahl 470 V/6 etc.

*References*
[1] W.D. Klotz, Computer Phys. Commun. 9 (1975) 102.
[2] W.D. Klotz, Computer Phys. Commun. 10 (1975) 70.

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* This work has been supported in part by the National Research Council of Canada.

* These decks can be replaced by AAHD; A NEW VERSION OF NJSYM; CPC 8 (1974) 151.

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# NUMERICAL SOLUTION OF KRAMERS–KRONIG TRANSFORMS BY A FOURIER METHOD

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Received 11 March 1977

## PROGRAM SUMMARY

*Title of program*: KRONIG

*Catalogue number*: ACMN

*Computer*: CDC CYBER 72-26; *Installation*: Computing Services Unit, University of New South Wales.

*Operating system*: KRONOS. 2.1.1 LEVEL 393

*Programming language used*: FORTRAN

*High speed storage required*: $31\mathrm{k}_8$

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer (unit 3) for testing.

*No. of cards in combined program and test deck*: 101

*Keywords*: Solid state physics, Kramers–Kronig, integral transform, magneto–optical activity, Fourier series.

*Nature of physical problem*
The two magneto–optical phenomena, the Faraday rotation and magnetic circular dichroism compose, respectively the real and imaginary parts of the complex optical rotation ($\hat{\phi} = \phi - \mathrm{i}\theta$). The Faraday rotation may then be calculated from the M.C.D. by use of the Kramers–Kronig integral relation [1]

$$\phi(\omega) = \frac{2}{\pi} \oint_0^\infty \frac{\Omega\, \theta(\omega)}{\Omega^2 - \omega^2}\, \mathrm{d}\Omega\ .$$

*Method of solution*
The solution utilizes the result [2] that if $\phi(\omega)$ and $\theta(\omega)$ are band limited (i.e. significantly non zero only within the frequency range $-\omega_1 < \omega < \omega_1$) then $\phi(\omega)$ and $\theta(\omega)$ can be written in terms of a fourier cosine series and Fourier sine series:

$$\phi(\omega) = 2 \sum_{m=1}^{\infty} b_m \cos(m\pi\omega/\omega_1)\ , \qquad (1)$$

$$\theta(\omega) = 2 \sum_{m=1}^{\infty} b_m \sin(m\pi\omega/\omega_1)\ . \qquad (2)$$

By finding values of $b_m$ that satisfy 2 and substituting these into 1 the values $\theta(\omega)$ are computed from $\phi(\omega)$. Each $b_m$ is calculated by a series method obviating the need for large storage and improving the speed of the calculation.

*Restrictions on the complexity of the problem*
The program computes $\phi(\omega)$ from $\theta(\omega)$ at equally spaced intervals where each and every M.C.D. data point is used to calculate the Fourier coefficient $b_m$. Currently the program is limited to 200 data points but this may be increased by modifying the program depending on available storage.

*Typical running time*
Typical running time on a CDC CYBER 72-26 for a transform with 200 data points is 14 sec.

*Unusual features of the program*
As the program uses a Fourier technique to compute the integral all problems concerning the Cauchy principal part encountered in numerical integration techniques are avoided. The program tests the accuracy of the method by using a gaussian function and comparing the calculated transform with that from theory, the gaussian having an exact analytic solution.

*References*

[1] C.A. Emeis et al., Proc. Roy. Soc. (London) 297A (1967) 54.
[2] D.W. Johnson, J. Phys. A. 8 (1975) 490.

Computer Physics Communication 13 (1977) 207–224
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# ELLIPS – A FORTRAN SIMULATION OF A POLARIZATION–MODULATION ELLIPSOMETER

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*Naval Research Laboratory, Washington, D.C. 20375, USA*

Received 3 November 1976

## PROGRAM SUMMARY

*Title of program*: ELLIPS

*Catalogue number*: ACXK

*Computer*: Texas Instruments ASC II, *Installation*: NRL

*Operating system*: OS4.021

*Programming language used*: FORTRAN IV

*High speed storage required*: 20 500 words

*No. of bits in a word*: 32

*Overlay structure*: none

*Peripherals used*: Card reader, printer

*No. of cards in combined program and test deck*: 1209

*Keywords*: Optics, ellipsometry, Jones matrices, polarization modulation, error analysis.

*Nature of the physical problem*
The problem treated is the analysis of the effect, on the detected AC signals, of imperfections in and misalignment of the optical components of a polarization–modulation ellipsometer. This permits correction of the values of $\psi$ and $\Delta$ (characteristics of the sample surface) for systematic error, estimation of the uncertainty in the final result, and identification of the most significant sources of experimental error.

*Method of solution*
The transmitted amplitude vector is computer using the Jones matrices of the individual components. The modified Jones matrices introduced by O'Handley [1] are used to separate the DC and AC components of the detected intensity.

*Typical running time*
1.4 sec for one datum point (systematic error correction with 5 iterations + complete calculations of experimental uncertainty). 0.3 sec for uncertainty calculation only.

*Reference*
[1] R.C. O'Handley, J. Opt. Soc. Am. 63 (1973) 523.

## ERRATUM NOTICES

*Title of manuscript*: Calculation of crystal potentials

*Authors*: D.A. Papaconstantopoylos and W.R. Slaughter

*Reference*: Computer Physics Communications 7 (1974) 207–214

*Title of program*: CRYSTAL POTENTIALS

*Catalogue number*: ACID

*Title of manuscript*: A new version of AAKF (reduced tensor matrix elements) adapted to spectroscopic notation.

*Authors*: C.F. Fischer and K.M.S. Saxena

*Reference*: Computer Phys. Commun. 9 (1975) 370

*Title of program*: REDUCED TENSOR MATRIX ELEMENTS 2

*Catalogue number*: AAKP

*Title of manuscript*: A program to evaluate the reduced matrix elements of summations of one-particle tensor operators

*Author*: W.D. Robb

*Reference*: Computer Phys. Commun. 6 (1973) 132

*Title of program*: REDUCED TENSOR MATRIX ELEMENTS

*Catalogue number*: AAKF

Computer Physics Communications 13 (1977) 251–269
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# CLASSICAL COLLISIONS OF PROTONS WITH HYDROGEN ATOMS

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N.A. VALENTINE
*Digital Equipment Corporation, Bilton House, Uxbridge Road, Ealing, London W.5., UK*

J.Mc.B. WILSON
*Department of Natural Philosophy, University of Glasgow, Glasgow W.2., Scotland, UK*

Received 24 June 1977

## PROGRAM SUMMARY

*Title of program*: CLASSICAL P–H COLLISIONS

*Catalogue number*: ACXO

*Computer*: CDC 6600

*Installation*: University of London Computing Centre.

*Operating system*: SCOPE 3.4

*Programming language used*: ASA FORTRAN

*High speed storage required*: 47 kwords (modifications are described which reduce the storage to 38 kw.)

*No. of bits in a word*: 60

*Overlay structure*: none.

*No. of magnetic tapes required*: none for the test run. Depends on the job.

*Other peripherals used*: none for the test run

*No. of cards in combined program and test deck*: 3060

*Keywords*: Atomic physics, classical, trajectory, collision, scattering, charge, body, electron, proton, hydrogen, Monte Carlo, cross section, ejection, energy transfer, representation, ionization, exchange, charge transfer, impact parameter, capture, rearrangement, state, inverse square, Runge–Kutta.

*Nature of physical problem*

The program solves the equations of motion for the interaction of 3 charged particles, obtaining final states in terms of initial states, and energy transfers, angles of ejection, and final cartesian co-ordinates of relative motion. Using a Monte Carlo method on many orbits total ionization and charge transfer cross sections, integral energy transfer cross sections and moments of energy transfers are estimated. Facilities are provided for obtaining angular distributions, momentum transfer cross sections and for comparison with various approximate classical theories.

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* Present address: Operations Research Unit, AERE Harwell, Oxfordshire OX11 0RA, U.K.

*Method of solution (1, 2, 3)*

The equations of motion are solved using stepwise fourth-order Runge–Kutta integration with automatic steplength change. Selection of initial conditions is determined by the user, usually as a statistical distribution determined by a pseudorandom number subroutine. Classical representation theory and transformation methods are extensively used.

*Restrictions*

Precise cross sections require considerable running time, particularly at low incident particle energies.

*Typical running time*

The test run takes approximately 0.3 s per orbit on a CDC 6600 for 50 keV protons incident on classical hydrogen atoms with 13.6 eV binding energy. For a given precision the time of integration increases approximately inversely with the velocity of the incident particle. An estimate of an ionization cross section at one energy in the neighbourhood of the maximum to within about 10% takes less than 2000 orbits. Energy transfer integral cross sections take longer by a factor of about 5.

Running time depends critically on careful use of the program, particularly impact parameter ranges and error parameters. The main references should be consulted before extensive use.

*Unusual features of the program*

Facilities are provided for storing essential orbit data on magnetic tape for later analysis, thus avoiding repeated numerical integrations.

The program is structured so that its size can be reduced, as shown in sec. 15.

*References*

[1] I.C. Percival. Comput. Phys. Commun. 6 (1973) 347.
[2] R. Abrines and I.C. Percival. Proc. Phys. Soc. 88 (1966) 861; 873.
[3] A. Burgess and I.C. Percival. Adv. Atom. Molec. Phys. 4 (1968) 109.

Computer Physics Communications 13 (1977) 271–280
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# FURI – A FORTRAN FUNCTION WRITER

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*Department of Physics, University of British Columbia, Vancouver, B.C., V6T 1W5, Canada*

Received 19 April 1977

## PROGRAM SUMMARY

*Title of Program*: FURI

*Catalogue number*: ACXP

*Computer*: IBM 370/168; *Installation*: University of British Columbia

*Operating system*: MTS/HASP

*High speed storage required*: 19.350K bytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, card punch

*No. of cards in combined program and test deck*: 632

*Keywords*: general purpose, polynomial fit, FORTRAN function writer.

*Nature of physical problem*
For the rapid evaluation of auxiliary functions required in physics, it is often advantageous to replace the function with a polynomial expansion or succession of polynomial expansions. This is a routine but tedious problem and should be automated.

*Method of solution*
The polynomial coefficients, evaluated from a table of data points in a standard fashion, are written out in the form of a FORTRAN statement. A self-contained FORTRAN function subroutine is generated by the program through the addition of standard control statements.

*Restrictions on the complexity of the problem*
The order of the sequence of polynomials is restricted to be from 1 to 8, from 2 to 8 if the slope is to be continuous, and to 3 for a spline fit.

*Typical running time*
2 s on IBM 370/168.

*Unusual features of the program*
The output consists of a function subroutine and a main program that is ready for testing the accuracy of the fit. By combining generated functions for different ranges of the independent variable, the user can put together a complete FORTRAN function program with a minimum of editing.

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Computer Physics Communications 13 (1977) 281–287
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# COUNTING A SMALL NUMBER OF RADIOACTIVE ATOMS

A.M. AURELA
*Wihuri Physical Laboratory, University of Turku, SF-20500 Turku 50, Finland*

Received 14 March 1977

## PROGRAM SUMMARY

*Title of program*: Counting few radioactive atoms

*Catalogue number*: AAUS

*Computer*: UNIVAC 1108 *Installation*: State Computer Centre, Helsinki.

*Operating system*: EXEC–8

*Programming language used*: ASA FORTRAN

*High speed storage required*: 25067 *words.*

*No. of bits in a word*: 36.

*Overlay structure*: none.

*No. of magnetic tapes required*: none.

*Other peripherals used*: Card reader and line printer

*No. of cards in combined program and test deck*: 123.

*Keywords*: Nuclear physics, radioactive decay, radioactive atoms, small sample, decays, statistical analysis, Bayesian analysis.

*Nature of physical problem*
The problem is to determine the frequency function $P(n)$ of the posterior probability that a small sample of a radioactive isotope $R$ contains $n$ atoms at the end of the production of $R$, when the counts in the subsequent counting periods are known.

*Method of solution*
First, $P(n)$ is computed for the beginning of the last counting period by a Bayesian method. Then $P(n)$ is used for computing a new $P(n)$ for the beginning of the preceding interval, if there was an interval. Then $P(n)$ is computed in the same way for the beginning of the preceding counting period, and so on. Mixed probability distributions are used for taking into account uncertainty in the efficiency and background rate of the detector.

*Restriction on the complexity of the probiem*
$n \leqslant 129$.

*Typical running time*
32 s (20 s CPU) on UNIVAC 1108.

*Unusual features of the program*
The repetitive application of Bayes's method to the multiple branches of possibilities, and the built-in a priori constraint $n \geqslant 0$, which reduces the error estimates.

Computer Physics Communications 13 (1977) 289–293
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# ADAPTATION OF THE NEW VERSION OF THE REDUCED TENSOR MATRIX ELEMENTS (AAKP) PROGRAM: INCLUSION OF THE EVALUATION OF MATRIX ELEMENTS OF TENSOR PRODUCTS *

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*Division of Theoretical Chemistry, Department of Chemistry, University of Alberta, Edmonton, Alberta, T6G 2G2 Canada*

Received 29 April 1977

## ADAPTATION SUMMARY

*Title of adaptation*: ADAPT TENSOR 2 FOR PRODUCT

*Adaptation number*: 0001

*Reference to the original Program*

*Title of program*: REDUCED TENSOR MATRIX ELEMENTS ‡

*Catalogue number*: AAKP

*Reference in CPC*: 9 (1975) 370

*Authors of original program*: C.F. Fischer and K.M.S. Saxena

*No. of Cards required to effect adaptation (including directive cards)*: 89

*CPC Library subprograms used*: Same as in the original program AAKP

*Additional keywords*: Tensor products, spin–dipolar interaction

*Purpose of the adaptation*

The program AAKP [1] is a new version (which uses spectroscopic notations for input/output purposes) of the program AAKF originally written by Robb [2]. Both these programs evaluate reduced matrix elements of the summations of one-particle tensor operators with respect to LS-coupled wavefunctions. The present adaptation makes it possible to use the program AAKP to evaluate the matrix elements (not reduced matrix elements) of a simple product of a spin-dependent tensor and a space-dependent tensor. A similar adaptation to AAKF has been recently published by Glass and Hibbert [3].

*References*

[1] C.F. Fischer and K.M.S. Saxena, Comput. Phys. Commun. 9 (1975) 370.
[2] W.D. Robb, Comput. Phys. Commun. 6 (1973) 132; 9 (1975) 268.
[3] R. Glass and A. Hibbert, Comput. Phys. Commun. 11 (1976) 125.

## ERRATUM NOTICE

*Title of manuscript:* Multistate molecular treatment of atomic collisions in the impact parameter approximation. II. Calculation of differential cross-sections from the transition amplitudes for the straight line case.

*Authors:* R.D. Piacentini and A. Salin

*Reference:* 13 (1977) 57

*Title of program:* EIKON

*Catalogue number:* ACXD

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* This work has been supported in part by the National Research Council of Canada.

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Computer Physics Communications 13 (1978) 323–340
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# FIFPC – A FAST ION FOKKER–PLANCK CODE *

R.H. FOWLER, J. SMITH and J.A. ROME
*Computer Sciences Division at Oak Ridge National Laboratory, Union Carbide Corporation, Nuclear Division, Oak Ridge, Tennessee 37830, USA*

Received 13 May 1977

## PROGRAM SUMMARY

*Title of program:* FIFPC

*Catalogue number*: ABSD

*Computer*: IBM 360/91; *Installation*: ORNL Computing Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830

*Operating system*: IBM system/360

*Programming language used*: FORTRAN IV

*High speed store required*: 270K bytes ($1105920_{10}$ words)

*No. of bits in a word*: 32 (8/byte)

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, Calcomp plotter (optional), CRT plotter (optional), disk or tape for plots (optional)

*No. of cards in combined program and test case*: 3936

*Keywords*: Plasma physics, Tokamak plasma, Fokker–Planck equation, distribution, fast ions, neutral beam injection

*Nature of physical problem*
The distribution function of fast ions resulting from neutral beam injection into a Tokamak plasma is calculated. The Fast Ion Fokker–Planck Code (FIFPC) also computes the momentum and power delivered to the electrons and ions in the background plasma, the power lost through charge exchange, the particle input to the plasma, and other quantities of interest.

*Method of solution*
FIFPC solves the Fokker–Planck equation [1] that describes the slowing down process of fast ions in a Tokamak plasma. This two-dimensional velocity space equation is transformed into sets of implicit finite difference equations to obtain the time-dependent solution or to obtain the steady-state solution directly. Two methods of solution are employed for the time-dependent problem. One method uses the Crank–Nicolson [2] scheme. The resulting set of finite difference equations is solved by using the strongly implicit procedure (SIP) developed by Stone [3]. The other method is based upon the alternating direction implicit (ADI) [4] scheme which results in equations with tridiagonal coefficient matrices that are solved using a standard technique [5]. The steady-state finite difference equations are solved by the SIP technique.

*Restrictions on the complexity of the problem*
FIFPC has been used over a large physical domain and has produced valid results for all cases with reasonable Tokamak parameters. The velocity space grid is limited to 40 points in each direction; however, this limit can be altered by changing the appropriate dimensions. The fast ions are assumed to stay on a flux surface and the pitch angle scattering operator for very untrapped ions is used. Thus, the code is most accurate for tangential injection and when the poloidal gyroradius is much less than the minor radius of the Tokamak.

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* Research sponsored by ERDA under contract with Union Carbide Corporation:

*References*

[1] J.G. Cordey and W.G.F. Core, Phys. Fluids 17 (1974) 1626.
[2] J. Crank and P. Nicolson, Proc. Camb. Philos. Soc. 43 (1947) 50.
[3] H.L. Stone, SIAM J. Numer. Anal. 5 (1968) 530.
[4] D.W. Peaceman and H.H. Rachford, Jr., J. Soc. Indust. Appl. Math. 3 (1955) 28.
[5] R.S. Varga, Matrix Iterative Analysis (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1962) p. 194.

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Computer Physics Communications 13 (1978) 341–348
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# CALCULATION OF THE FIRST DERIVATIVES OF MADELUNG CONSTANTS WITH RESPECT TO CELL LENGTHS

H.D.B. JENKINS and K.F. PRATT
*University of Warwick, Conventry, W. Midlands, CV4 7AL, UK*

Received 23 May 1977

## PROGRAM SUMMARY

*Title of program*: MADELUNG DERIVATIVES

*Catalogue number*: ACMO

*Computer*: B6700; *Installation*: Computer Centre, University of Warwick, Coventry, W. Midlands, CV4 7AL.

*Operating system*: Master Control Program

*Programming language used*: FORTRAN IV

*High speed storage required*: 6 500 words

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader lineprinter and/or on-line terminal

*No. of cards in combined program and test deck*: 1099

*Reference to other published version of this program*: QCPE Program 222

*Keywords*: Solid state physics, Madelung constant, Madelung derivatives, Bertaut method, Fourier transform, complex ion, self energy.

*Nature of physical problem*
To calculate the Madelung constant and its derivatives with respect to the cell lengths for the input crystal structure, in a charge dependent and charge independent form.

*Method of solution*
The Madelung constant is calculated by the use of the Bertaut [1] approach. This is differentiated term by term to obtain the derivatives with respect to the cell lengths. Complex ions can be treated as entities having fixed geometry and if this is done their self energy may be calculated.

*Restriction on the complexity of the problem*
The cut-off radius of the charge-density function must be chosen as cell length independent.
If a Gaussian charge-density function is used and an overlap correction is required then derivatives will not be calculated.

*Typical running time*
For sodium nitrite ($NaNO_2$) [2] with convergence to six decimal places [3]–1000 s.

*References*

[1] E.F. Bertaut, J. Phys. Radium 13 (1952) 499.
[2] M.I. Kay and B.C. Frazer, Acta Cryst. 14 (1961) 56.
[3] H.D.B. Jenkins, Chem. Phys. Lett. 9 (1971) 473; 20 (1973 155;
H.D.B. Jenkins, J. Chem. Soc. Faraday II, 72 (1976) 1569.

Computer Physics Communications 13 (1978) 349–362
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# A LINEAR ACCELERATOR CAVITY CODE BASED ON THE FINITE ELEMENT METHOD

A. KONRAD
*National Research Council, Ottawa, Ontario, Canada*

Received 14 February 1977

## PROGRAM SUMMARY

*Title of program*: LINEAR ACCELERATOR CAVITY CODE

*Catalogue number*: ACSK

*Computer*: IBM 360/75

*Installation*: McGill University Computing Centre, Montreal, Canada

*Computer*: IBM 360/67

*Installation*: National Research Council Computing Centre, Ottawa, Canada

*Operating System*: IBM System/360 Time Sharing System

*Programming language*: FORTRAN IV

*High speed storage required*: 75 K words

*No. of bits in a word*: 32

*Overlay structure*: 1) MAIN 2a) READIN, MAP
2b) FINDIT
2c) ASSEMB, LOCATE, ROTAT1, ROTAT2, FLIP, TWSFL1, TWSFL2, ONE, TWO, BLOCK1, BLOCK2, BLOCK3, BLOCK4, BLOCK5
2d) EIGVAL
2e) EIGVEC
2f) DERIV, BLOKK1
2g) AINTEG
2h) COTES1, COTES2, BLOKK2, BLOKK3
2i) LINAC
2j) OUTPUT

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, card punch (optional), two temporary disc files

*No. of cards in combined program and test deck*: 6193

*CPC library subprograms used (optional)*:

*Catalogue number*: ACSF

*Title*: VECTR-FINTEL6-BLK-DATA-GENERATOR

*Ref. in CPC*: 9 (1975) 193

*Keywords*: Nuclear physics, Linear accelerator, Linac cavity, Axisymmetric, Vector field, Finite element, electromagnetics

*Nature of physical problem*
The program solves the classical electromagnetic field problem of the empty, axially symmetric resonator with conducting walls [1]. The solution of this problem is of major importance to linear accelerator cavity designers who need to obtain performance measuring quantities from the magnetic field distribution in the cavity.

*Method of solution*
The program algorithm is based on a variational formulation coupled with the high-order polynomial, triangular finite element method for the magnetic field calculation [1]. Various other numerical methods such as one- and two-dimensional Newton-Cotes integration are used to obtain the performance measuring quantities (e.g. transit time factor, stored energy, power loss, shunt impedance, $Q$-factor).

*Unusual features of the program*

The program is a double precision, specialized version of the AXISYMM-VECTOR-HELMHOLTZ-FINTEL6 computer program [2] and has the same unusual features (e.g. the five block data subprograms BLOCK1 through BLOCK5). Users of other than IBM computers must use the VECTR-FINTEL6-BLK-DATA-GENERATOR program [2] to generate block data compatible with their FORTRAN compilers.

*References*

[1] A. Konrad, IEEE Trans. Nucl. Sci. NS-20 (1973) 802.
[2] A. Konrad and P. Silvester, Commun. 9 (1975) 193.

Computer Physics Communications 13 (1978) 363–370
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# THE COMPUTATION OF STEADY STATE ARCS IN NOZZLE FLOW

M.T.C. FANG, S.K. CHAN * and R.D. WRIGHT
*Department of Electrical Engineering and Electronics, University of Liverpool, UK*

Received 8 July 1977

## PROGRAM SUMMARY

*Title of program*: DCANF

*Catalogue number*: ABUS

*Computer*: *Installation*:
CDC7600/ICL1906A University of Manchester, Regional Computer Centre

*Operating system*: Scope 2.1.

*Programming language used*: FORTRAN

*High speed storage used*: 12000 words

*Number of bits in a word*: 60 bits

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader; line printer.

*No. of cards in combined program test deck*: 931

*Keywords*: arc, plasma physics, electric, gas flow, thermal plasma, nozzle

*Nature of physical problem*
DCANF finds the supercritical solution of a high pressure arc burning in a converging–diverging nozzle where the primary standard shape factors [1,2] are assumed constant and the external flow one-dimensional.

*Method of solution*
The three first-order ordinary differential equations, $[Q]\,\mathrm{d}x/\mathrm{d}\zeta = b$ [1], describing the d.c. arcs in nozzle flow are solved for a given solution parameter, $K$ assuming constant standard primary shape factors [2]. To obtain the supercritical solution, it is necessary to ensure that $|Q| = 0$ and the compatibility conditions are satisfied simultaneously at the critical point, $\zeta_c$. This is ensured by guessing the arcing conditions at the critical point (i.e. the velocity magnitude factor $g_c$ and $\beta_c$, the ratio of the arc displacement area to the nozzle area). The governing equations are integrated forward from the upstream electrode and backward from the critical point to the socalled patching point. The sum of the squares of the differences of the dependent variables at the patching point is then minimised with respect $g_c$ and $\beta_c$ using Powell's method [3].

*Typical running time*
With reasonable guesses for $g_c$ and $\beta_c$, a solution can usually be found within 1.5 s on CDC7600.

*References*

[1] S.K. Chan, M.T.C. Fang and M.D. Cowley, University of Liverpool, Dept. of Elec. Eng., Arc Research Project Report No. ULAP-T.44.
[2] S.K. Chan, M.D. Cowley and M.T.C. Fang, J. Phys. D. 9 (1976) 1085.
[3] M.J.D. Powell, Comp. J. 7 (1964) 155.

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* Engineering Department, Cambridge University. Now at: Mechanical Engineering Department, University of Hong Kong, Hong Kong.

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# DBLCON: A VERSION OF POSITRONFIT WITH NON-GAUSSIAN PROMPT FOR ANALYSING POSITRON LIFETIME SPECTRA

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*Div. Engineering & Appl. Physics, Harvard University, Cambridge, Massachusetts, 02138 USA*

Received 20 July 1977

## PROGRAM SUMMARY

*Title of program*: DBLCON

*Catalogue number*: AAGZ

*Computer*: PDP 10, IBM 370/165 [*]; *Installation*: Brandeis University, Waltham, MA. 02154 USA; M.I.T., Cambridge, MA. 02139 USA

*Operating system*: Disk

*Programming language used*: FORTRAN IV

*High speed storage required*: 39 K words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: none

*No. of cards in combined program and test deck*: 1336

*References to other published versions of this program*:
*Catalogue number*: AAGK; *Title*: POSITRONFIT
*Ref. in CPC*: *3* (1972) 240.

*Keywords*: Atomic, nuclear, positron, lifetime, time spectrum, least-squares, fitting, convolution, minimization, sum-of-exponentials, iterations, Marquardt, constraints, covariance matrix.

*Nature of physical problem*
Analysis of positron lifetime spectrum assuming a non-Gaussia spectrometer resolution function.

*Method of solution*
Least-squares technique [1].

*Restrictions on the complexity of the problem*
Two exponentials required for the prompt, a maximum of three allowed in the spectrum. No independent source correction is included.

*Typical running time*
Analysis of a typical lifetime spectrum requires about 20 s of CPU time on the PDP 10.

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[*] With minor changes.

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# COMPUTATION OF PHONON SPECTRUM FROM THE COLD NEUTRON INCOHERENT INELASTIC SCATTERING BY A POLYCRYSTAL

T.D. SOKOLOVSKIJ and L.A. ROGOSCHENKO
*Institute of Physics of Solids and Semiconductors, Minsk, USSR*

Received 19 April 1977

## PROGRAM SUMMARY

*Title of program*: RESTOR 1

*Catalogue number*: ACXT

| *Computer*: | *Installation*: |
|---|---|
| EC 1030,<br>IBM 360; | Computer Center, Institute of Mathematics,<br>Academy of Sciences, Minsk, 220726, USSR |

*Operating system*: DOS

*Programming language used*: FORTRAN IV

*High speed storage required*: 80 (octal) words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, printer

*No. of cards in combined program and test deck*: 246

*Keywords*: solid state, phonon spectrum, incoherent, inelastic, scattering, cold neutron, monocrystal, polycrystal

*Nature of the physical problem*
RESTOR 1 computes the phonon spectrum from the incoherent inelastic scattering data of cold neutrons by a polycrystal consisting of identical atoms.

*Method of solution*
A nonlinear integral equation for the phonon frequency distribution in a polycrystal is constructed. This equation is solved by the method of consecutive approximations.

*Restrictions on the complexity of the problem*
The program is limited to polycrystals with identical atoms. It is assumed that the neutrons are scattered with energy gain. But the program RESTOR 1 provides for the case of scattering with energy loss, when the factor $\exp\{\epsilon/k_B T\}$ appears on the right-hand side of eq. (4) in the long write-up.

*Typical running time*
The time required for the test run is 4 min 30 s on the EC 1030 computer, of which 2 min is taken in compiling.

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# UPEAK – SPECTRO-ORIENTED ROUTINE FOR MIXTURE DECOMPOSITION

V.B. ZLOKAZOV
*Joint Institute for Nuclear Research, Head Post Office, PO Box 79, Moscow, USSR*

Received 4 February 1977

## PROGRAM SUMMARY

*Title of program*: UPEAK

*Catalogue number*: ABAA

| *Computer*: | *Installation*: |
|---|---|
| CDC - 6500 | JINR, Laboratory of Computing technique and Automation, Dubna |

*Operating system*: SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: 32 k words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, card punch (optional)

*No. of cards in combined program and test deck*: 4406

*Keywords*: Nuclear, molecular, spectrum, emission, absorption, mixture decomposition, regression analysis, spectrum analysis, spectrometry, data processing

*Nature of physical problem*
The program decomposes one-dimensional spectra of nuclear or molecular emission (absorption) into the components of interest and those of background, and evaluates such quantities as positions, areas and widths of the components of interest.

*Method of solution*
The program inputs the models of the components of interest and that of background, which may be constructed using either analytical functions, describing the component shape, or experimentally measured histograms, representing that shape, and fits the spectrum (divided into parts), estimating the characteristics of the relations between the models and the real images in such a way that these estimates determine at the same time the values of quantities of interest: position, area, width (fwhm).

*Restrictions on the complexity of the problem*
The maximum number of components in the analyzed spectrum interval = 20; not more than 2 different models of components of interest per spectrum interval may be employed.

*Typical running time*
Essentially depends on: 1) amount of output data to be printed; 2) number of channels in the interval; 3) presence and extent of overlap and (or) of weakness of the components; the "average case" takes about 1 s per component.

*Unusual features of the program*
The input–output is organized such that the program is able to be a module inside an external program or to run as an independent routine.

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# MONTE CARLO INTEGRATION PROGRAM FOR THE *n*-PARTICLE RELATIVISTIC PHASE SPACE INTEGRAL IN INVARIANT VARIABLES *

Richard A. MORROW,
*Bennett Hall, University of Maine, Orono, Maine 04473, USA*

Received 9 June 1977

## PROGRAM SUMMARY

*Title of program*: MCN

*Catalogue number*: AAWB

*Computer*: IBM 370/148; *Installation*: University of Maine, Orono, Maine 04473

*Operating system*: CMS (G compiler) or DOS (F compiler)

*Programming language used*: FORTRAN IV

*High speed storage required*: 31,000 words

*No. of bits in a word*: 32

*Overlay structure*: not used

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader; line printer

*No. of cards in combined program and test desk*: 600

*Keywords*: Nuclear physics, high energy, elementary particle, multiparticle, Monte Carlo, phase space, Lorentz invariants, physical region, exceptional regions, importance sampling, cross section, differential distribution, scatter plot.

*Nature of physical problem*
In scattering and production reactions of relativistic elementary particles, cross sections and differential distributions resulting from an assumed theoretical transition matrix element are often wanted. The *n*-particle relativistic momentum phase space integral must be numerically evaluated to yield such information. In the course of this evaluation not only are $3n$-10 independent variables dealt with but, in general, several dependent variables are encountered as well.

*Method of solution*
A Monte Carlo integration method is used to numerically evaluate the phase space integral by randomly generating values of the independent variables [1]. Subsequently several dependent invariants which depend on the independent ones in a nonlinear fashion are evaluated. The invariant variables used are squares of sums of adjacent 4-momenta. Facilities are also provided for the printing out of desired distributions in both tabular and histogram form.

*Restrictions on the complexity of the problem*
The program is dimensioned for up to 15 (incoming plus outgoing) particles, for up to 24 distributions and for up to 5 scatter (two dimensional) plots. Each of the 24 distributions can have up to 100 bins. Any or all of these limits can be easily increased by the user.

*Unusual features of the program*
MCN is unique in the manner in which the dependent invariants are calculated from randomly generated values of the independent ones. A rapid, direct, iterative method is used which is accurate even in the exceptional regions of the

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* Work supported in part by a Faculty Summer Research award from the University of Maine at Orono.

physical region, eg. those regions corresponding to forward-like scattering. Another unusual feature is that the first distribution printed out is actually a test distribution that serves to indicate how efficient the event generation has been. Details of the analytical work underlying this program can be found elsewhere [2].

*References*

[1] E. Byckling, M. Kaartinen, K. Kajantie and H. Villanen, J. Comput. Phys. 4 (1969) 521.

[2] R.A. Morrow, "Algorithm for the Numerical Evaluation of the $n$-particle phase space integral in invariant variables University of Maine at Orono preprint.

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# SIMULATION OF THERMALLY STIMULATED DIPOLAR PROCESSES IN DIELECTRICS

A. LINKENS, J. VANDERSCHUEREN *
*Department of Physical Chemistry, University of Liège, Sart-Tilman, B4000 Liège, Belgium*

P. PAROT and J. GASIOT
*Centre d'Etude d'Electronique du Solide, Place Eugène Bataillon, 34000 Montpellier, France*

Received 3 August 1977

## PROGRAM SUMMARY

*Title of program*: TSP

*Catalogue number*: ACKP

*Computer*: MODCOMP II, or IBM 370/158; *Installation*: University of Liège

*Operating system*: MAX II Release ULG 0.4.1 (or VS2-R01.6)

*Program language used*: FORTRAN IV

*High speed storage required*: 11k bytes on Modcomp II or 64k bytes on IBM 370/158

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: optional

*Other peripherals used*: papertape – or card-reader, lineprinter, 1 or 2 sequential scratch files

*No. of cards in combined program and test deck*: 497

*Keywords*: Solid state physics, simulation, thermal stimulation, polarization, depolarization, dipolar polarization, relaxation time, activation energy.

*Nature of physical problem*
Program TSP simulates the phenomena produced in a solid dipolar sample submitted to thermal cycles while in an external electric field. Dipolar orientation and thermal randomization are the two competing effects, the relative importance of which varies with the field, the actual temperature and the thermal history of the sample (i.e. the previous thermal cycles). The polarization, and the displacement current showing changes in the polarization, are computed by TSP to support theoretical predictions and to help experimental interpretation.

*Method of solution*
The differential equation of the detailed balance is integrated to compute the polarization. The current is obtained by taking the derivative of the polarization at the time.

*Typical running time*
Without plot feature for short test data MODCOMP II : 102 s, or IBM 370/158 : 14 s.

*Restrictions on the complexity of the problem*
The number of successive thermal cycles is limited to 6. Unless sizes of 4 vectors are changed, the job must not simulate thermal cycles extended over more than 600 seconds.

*Unusual features of the program*
None in the Fortran statements. On Modcomp II, we use a plot feature (see TTOP below) that can be deleted by just suppressing one instruction (subroutine call) in the deck.

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* Chargé de Recherches of the Fonds National de la Recherche Scientifique (Belgium). J. Vander Schueren is the third author, and P. Parot the second.

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Computer Physics Communications 13 (1978) 421–427
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# A FORTRAN PROGRAM TO COLLECT HISTOGRAMS OF MICROSCOPIC SCALAR INTERACTIONS

E.D. von MEERWALL
*Physics Department, The University of Akron, Akron, Ohio 44325, USA*

Received 10 October 1977

## PROGRAM SUMMARY

*Title of program*: INTHIST2

*Catalogue number*: ABMX

*Computer*: IBM 370/158; *Installation*: The University of Akron, Akron, Ohio 44325, USA

*Operating system*: OS/MVT; OS/VS2; OS/MVS

*Programming language used*: FORTRAN IV (G)

*High-speed store required*: 10,000 words (40 kbt) exclusive of loader

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 729

*Keywords*: Solid state physics, simulation, histogram, microscopic interaction, nuclear magnetic resonance, lattice, impurity, metal, disordered alloy.

*Nature of physical problem*
The effects of scalar interactions among members of a host lattice, and/or between these and an interstitial or substituted species, are simulated.

*Method of solution*
The interactions depending on distance (and perhaps also direction) between a subject location and a finite set of object points are added. This procedure is repeated for all subject points within their limits and the results accumulated in a histogram, and plotted.

*Restrictions on program complexity*
There are no limits on the number of subject lattice points; the limits of 400 on the number of a second species, and of 100 on the number of histogram boxes, are easily extended.

*Typical running time*
On the IBM 370/158, the program compiles (FORTRAN IVG in about 9 CPU seconds. Interactions between about 10,000 subject atoms and up to 400 impurity atoms take about 30 CPU seconds; including the intraspecies interactions increases processing time by an order of magnitude.

*Unusual features of the program*
(1) The subject lattice may be simple, bc or fc cubic, tetrahedr or orthorhombic; locations are created dynamically during the calculations;
(2) an optional second species may be created either by random substitution (lattice as above) or by input of individual coordinates; interactions may be confined to specifie fractions of each population;
(3) without recompilation, the program may access any of three types each of intraspecies and interspecies interaction; their parameters are supplied with each case;
(4) the program as supplied is appropriate for NMR spectral lineshapes in metals and disordered alloys; modifications for other uses and non-scalar interactions should be minimal.

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# ERRATUM NOTICE

*Title of manuscript:* A general program to calculate angular momentum coefficients in relativistic atomic structure

*Authors:* I.P. Grant

*Reference:* Comp. Phys. Commun. 5 (1973) 397.

*Title of program:* MCP

*Catalogue number:* ACRJ

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# A COMPACT PROGRAM OF THE SCF-X$\alpha$ SCATTERED WAVE METHOD

S. KATSUKI, P. PALTING and S. HUZINAGA
*Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada*

Received 19 April 1977

## PROGRAM SUMMARY

*Title of program*: MSXALPHA

*Catalogue number*: ACXN

*Computer*: Amdahl 470V/6; *Installation*: University of Alberta, Edmonton, Alberta, Canada

*Operating system*: MTS

*Programming language used*: FORTRAN IV

*High speed core required*: 438 K bytes

*Number of bits in a byte*: 8

*Overlay structure*: none

*Number of magnetic tapes required*: one or none

*Other peripherals required*: card reader, line printer, disk

*Number of cards in the combined program and test deck*: 6255

*Keywords*: Quantum chemistry, molecular, structure, orbitals, energy levels, muffin-tin approximation, non-overlapping spheres, X$\alpha$ approximation, initial atomic orbitals, ground state, transition state

*Nature of physical problem*
The present program calculates molecular orbitals and energy levels by solving the MSX$\alpha$ equations in the muffin-tin approximation for the case of non-overlapping contingent spheres [1]. These calculations are done for the ground-state configuration and transition-state theory is used to compute electronic transitions [2–4].

*Method of solution*
Initial atomic orbitals are used to generate the potential in the X$\alpha$ approximation with appropriate division of the molecular space into spherical regions. Radial Schrödinger equations are solved by the Runge–Kutta–Milne method in the spherical atomic regions and the extra molecular region. Energy eigenvalues and eigenvectors for the interatomic regio are obtained from determining the zeros of the secular determinant with the aid of the Gaussian elimination method with complete pivoting. Special procedures are used to distinguish zeros from poles and to speed up the calculation of these zeros in subsequent iterations. With the newly found molecular orbitals the procedure of determining the potential, eigenvalues, and molecular orbitals is repeated until the eigenvalues convergence.

*Restriction on the complexity of the problem*
The present version of the program handles only the spin-restricted case.

*Typical running time*
The CPU time required for the calculation mentioned in the test run was about 3 min on the Amdahl 470V/6.

*Unusual features of the program*
The present version of the program permits one to use analyt Hartree–Fock orbitals in an STO or GTO basis or numerical orbitals as the initial atomic orbitals. Provision is made to do a calculation piece-wise and to make restarts from a given iteration. Core orbitals may be frozen during a calculation. Once valence levels are well behaved, they are automatically treated as core-like orbitals; this provision speeds up the search for zeros of the secular determinant and here reduces the time consumed for each iteration.

*FORTRAN compatibility*

The present program is written in IBM FORTRAN IV. The following features used in the program may not be compatible with other FORTRAN languages:

(1) arrays COEFF and DZT are four-dimensional;
(2) apostrophes are used in Format statements to define hollerith strings instead of the standard field description nH;
(3) array element expressions which involve more than one variable or another array element are used, e.g.
SYMOVL(I2 + IW, ),
NDG(IRG3(I));
(4) IMPLICIT REAL*8 and COMPLEX*16 are used;
(5) characters, ϵ and #, are used in column 6 for continuation lines which may possibly cause problems on other computers, and
(6) the ENTRY statement is used.

*References*

[1] K.H. Johnson, Advan. Quantum Chem. 7 (1973) 143.
[2] J.C. Slater, in: Computational Methods in Bond Theory, P.M. Marcus, J.F. Janak, and A.R. Williams, eds. (Plenum Press, New York, 000) p. 447.
[3] J.C. Slater, Advan. Quantum Chem. 6 (1972) 1.
[4] J.C. Slater and K.H. Johnson, Phys. Rev. B5 (1972) 844.

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Computer Physics Communications 14 (1978) 71–79
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# DIAGRAMMATIC MANY-BODY PERTURBATION EXPANSION FOR ATOMS AND MOLECULES: I. GENERAL ORGANIZATION

David M. SILVER
*Applied Physics Laboratory, The Johns Hopkins University, Laurel, Maryland 20810, USA*

Received 1 September 1977; in revised form

## PROGRAM SUMMARY

*Title of program*: MBPT ORGANIZATION

*Catalogue number*: ACXF

*Computer*: IBM 360/91; *Installation*: The Johns Hopkins University Applied Physics Laboratory

*Operating system*: ASP

*Programming language*: FORTRAN IV

*High speed storage required*: 200 kilobytes

*Number of bits in a byte*: 8

*Overlay structure*: 7 segments, 3 nodes

*Number of magnetic tapes required*: none

*Other peripherals used*: disc drives, line printer, card reader

*Number of cards in combined program and test deck*: 1454

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACXG | MBPT LADDER DIAGRAMS | 13 (1978) this issue |
| ACXH | MBPT RING DIAGRAMS | 13 (1978) this issue |

*Keywords*: quantum chemistry, atomic, molecular, electronic, structure, diagram, many-body, perturbation theory, Padé approximant

*Nature of physical problem*
The determination of perturbative solutions to the non-relativistic Schrödinger equation for the electronic structure of atomic and molecular systems is considered within the Born–Oppenheimer approximation.

*Method of solution*
The diagrammatic many-body perturbation expansion is employed through third-order in the energy and first-order in the wavefunction, including all many-body effects that arise. The calculations are performed within the algebraic approximation in which eigenfunctions are parameterized by expansion in a finite set of basis functions. Computer algorithms are presented for the organization and sorting of the one-electron and two-electron interaction integrals; and the calculation of final results, including Padé approximants and variational many-body perturbative upper-bounds to the energy eigenvalue.

*Restrictions on the complexity of the problem*
These programs are restricted to non-degenerate, closed-shell ground-states of atoms and molecules. The reference wavefunction must be a closed-shell matrix Hartree–Fock single-determinantal wavefunction. Program dimension statements limit the basis set size to 10 occupied spatial orbitals (20 electrons) and 25 unoccupied spatial orbitals (50 virtual states): these dimensions can easily be increased if necessary.

*Typical running time*
Running times depend strongly on the basis set size and on the number of occupied orbitals: some timing data have been presented [1,2]. The test run requires ~1.5 s of CPU time on the IBM 360/91 for the subprograms within the domain of this paper.

*Unusual features of the program*
This program is an integral part of a set of programs [3,4]. This program prepares the input to the other parts of the set and uses the output from those routines to calculate the final results.

*References*

[1] S. Wilson and D.M. Silver, Phys. Rev. A14 (1976) 1949.
[2] S. Wilson and D.M. Silver, J. Chem. Phys. 67 (1977) 5400.

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[3] D.M. Silver, Comput. Phys. Commun. 14 (1978) 81.

[4] S. Wilson, Comput. Phys. Commun. 14 (1978) 91.

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# DIAGRAMMATIC MANY-BODY PERTURBATION EXPANSION FOR ATOMS AND MOLECULES: II. SECOND-ORDER AND THIRD-ORDER LADDER ENERGIES

David M. SILVER
*Applied Physics Laboratory, The Johns Hopkins University, Laurel, Maryland 20810, USA*

Received 1 September 1977; in revised form

## PROGRAM SUMMARY

*Title of program*: MBPT LADDER DIAGRAMS

*Catalogue number*: ACXG

*Computer*: IBM 360/91; *Installation*: The Johns Hopkins University Applied Physics Laboratory

*Operating system*: ASP

*Programming language*: FORTRAN IV

*High speed storage required*: 200 kilobytes

*Number of bits in a byte*: 8

*Overlay structure*: 4 segments, 1 node

*Number of magnetic tapes required*: none

*Other peripherals used*: disc drives, line printer.

*Number of cards in combined program and test deck*: 794

*CPC Library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACXF | MBPT ORGANIZATION | 14 (1978) this issue |
| ACXH | MBPT RING DIAGRAMS | 14 (1978) this issue |

*Keywords*: quantum chemistry, atomic, molecular, electronic, structure, diagram, many-body, perturbation theory, ladder diagram

*Nature of physical problem*
The determination of perturbative solutions of the non-relativistic Schrödinger equation for the electronic structure of atomic and molecular systems is considered within the Born-Oppenheimer approximation.

*Method of solution*
The diagrammatic many-body perturbation expansion is employed through third-order in the energy and first-order in the wavefunction, including all many-body effects that arise. The calculations are performed within the algebraic approximation [1] in which eigenfunctions are parameterized by expansion in a finite set of basis functions. Computer algorithms are presented for the evaluation of second-order energies; overlap integrals over the first-order perturbative wavefunction; and third-order particle–particle and hole–hole ladder diagrams.

*Restrictions on the complexity of the problem*
These programs are restricted to non-degenerate, closed-shell ground-states of atoms and molecules. The reference wavefunction must be a closed-shell matrix Hartree–Fock single-determinantal wavefunction. Program dimension statements limit the basis set size to 10 occupied spatial orbitals (20 electrons) and 25 unoccupied spatial orbitals (50 virtual states): these dimensions can easily be increased if necessary.

*Typical running time*
Running times depend strongly on the basis set size and on th number of occupied orbitals: some timing data have been presented [1,2]. The test run requires ~0.6 s of CPU time on the IBM 360/91 for the subprograms within the domain of this paper.

*Unusual features of the program*
This program is an integral part of a set of programs [3,4]. This program requires input from a previous part of the set and returns its output to those routines [3].

*References*

[1] S. Wilson and D.M. Silver, Phys. Rev. A14 (1976) 1949.
[2] S. Wilson and D.M. Silver, J. Chem. Phys. 67 (1977) 5400.
[3] D.M. Silver, Comput. Phys. Commun. 14 (1978) 71.
[4] S. Wilson, Comput. Phys. Commun. 14 (1978) 91.

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# DIAGRAMMATIC MANY-BODY PERTURBATION EXPANSION FOR ATOMS AND MOLECULES:
## III. THIRD-ORDER RING ENERGIES

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Received 1 September 1977; in revised form

## PROGRAM SUMMARY

*Title of program*: MBPT RING DIAGRAMS

*Catalogue number*: ACXH

*Computer*: IBM 360/91

*Installation*: The Johns Hopkins University Applied Physics Laboratory

*Operating system used*: ASP

*Programming language*: FORTRAN IV

*High speed storage required*: 200 kilobytes

*Number of bits in a byte*: 8

*Overlay structure*: 6 segments, 2 nodes

*Number of magnetic tapes required*: none

*Other peripherals used*: disc, line printer, card reader

*Number of cards in combined program and test deck*: 739

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACXF | MBPT ORGANIZATION | 14 (1978) this issue |
| ACXG | MBPT LADDER DIAGRAMS | 14 (1978) this issue |

*Keywords*: quantum chemistry, atomic, molecular, electronic, structure, diagram, many-body, perturbation theory, third-order, hole–particle diagram, ring diagram.

*Nature of the physical rpoblem*
The non-relativistic Schrödinger equation for the electronic structure of atomic and molecular systems is considered within the Born–Oppenheimer approximation.

*Method of solution*
The diagrammatic many-body perturbation expansion is employed through third-order in the energy and first-order in the wave function. All many-body terms are evaluated. The calculations are performed within the algebraic approximation [1] in which the one-electron state functions are parameterized by expansion in a finite set of basis functions. Computer algorithms are presented for the evaluation of third-order hole–particle, or ring, diagrams.

*Restrictions on the complexity of the problem*
The reference wave function must be a non-degenerate, closed-shell Hartree–Fock determinant. The current program is restricted to systems containing up to twenty electrons described by basis sets containing a maximum of 35 spatial functions. These latter restrictions are easily changed.

*Typical running time*
Running times are strongly dependent on the size of the basis set and the number of electrons. Some timing data has been presented previously [1,2]. The test run requires 1.5 s of of CPU time on an IBM 360/91 computer for the execution of the subprograms described in this paper.

*Usual features of the program*
This program is designed for use with those described in the two preceding papers [3,4].

*References*
[1] S. Wilson and D.M. Silver, Phys. Rev. A14 (1976) 1949.
[2] S. Wilson and D.M. Silver, J. Chem. Phys. 67 (1977) 5400.

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[3] D.M. Silver, Comput. Phys. Commun. 14 (1978) 71.

[4] D.M. Silver, Comput. Phys. Commun. 14 (1978) 81.

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Computer Physics Communications 14 (1978) 99–107
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# A PROGRAM FOR CALCULATING ELASTIC SCATTERING PHASE SHIFTS FOR AN ELECTRON COLLIDING WITH A ONE-ELECTRON TARGET USING PERTURBATION THEORY

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*The Queen's University of Belfast, Belfast, BT7 1NN, Northern Ireland*

Received 15 September 1977

## PROGRAM SUMMARY

*Title of program*: LAG 1

*Catalogue number*: ACYD

| *Computer*: | *Installation*: |
|---|---|
| ICL 1906S | Queen's University of Belfast Computer Centre |

*Operating system*: GEORGE 4 (BOSS)

*Programming language used*: FORTRAN IV

*High speed storage required*: 96 Kwords

*No. of bits in a word*: 24

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1587

*Keywords*: Atomic, scattering, coupled differential equations, electron, frozen-core, Hartree-Fock, long range potential, perturbation, phase shift, Slater-type orbital, WBK, wave function, one-electron atom

*Nature of physical problem*

In calculating elastic scattering phase shifts in electron-atom scattering it is important to take adequate account of the correlation between the colliding electron and the target electrons which is not included in the static-exchange appro imation. This can be achieved using perturbation theory. Thi program calculates elastic scattering phase shifts for $e^- + A($ scattering, where A(1) is a one-electron target, and is applicable for any collision energy $<\frac{3}{4}z^2$, and any angular momen tum and any total spin.

*Method of solution*

Perturbation theory based on the frozen-core-Hartree-Fo approximation in zero-order is used to calculate corrections to the F.C.H.F. phase shifts. See [1] and [2].

*Typical running time*

The main factors controlling the running time are the number of exponent values being considered for the particular collision energy and the size of the $Q$-space wave functio representation. Generally 100 seconds should be allowed fo each value of the exponent.

*References*

[1] K. Smith, The Calculation of Atomic Collision Processe (Wiley–Interscience, New York, 1971).
[2] A.L. Stewart, J. Phys. B: Atom. Molec. Phys., Vol. 10, No. 11, 1977.

Computer Physics Communications 14 (1978) 109–120
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# REDUCED SU(3) CFP's *

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Received 7 July 1977

## PROGRAM SUMMARY

*Title of program*: REDUCED SU(3) CFPS

*Catalogue number*: ABKG

| *Computer*: | *Installation*: |
|---|---|
| AMDAHL 470V/6<br>IBM 360; | Univ. Michigan, Ann Arbor, Michigan |

*Operating System*: MTS

*Program language used*: FORTRAN

*High speed storage required*: 197k words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 3655

*CPC Library data deck used*:
Catalogue number: AAC*; Title: DATA FOR ABKG

*No. of cards in data deck*: 7423

*Keywords*: Nuclear physics, theoretical methods, CFP, SU(3), SU(4), shell model, spectroscopic amplitude, $\alpha$-transfer, pseudo-SU(3).

*Nature of physical problem*
Reduced SU(3) $x$-particle coefficients of fractional parentage (CFP) are calculated, for any nuclear shell and arbitrary shell model states in an SU(3) × SU(4) or an SU(3) × SU(2) scheme. These CFP together with the SU(3) coupling coefficients available with the code of ref. [1] make it possible to perform standard shell model calculations in the SU(3) scheme.

*Method of solution*
Raising and lowering operators of SU(3) and SU(4) are used to construct explicitly shell model states of good SU(3) × SU(4) symmetry [2]. These states are written in terms of Fermion creation operators. Overlaps can then be calculated directly and lengthy recursion is thus avoided.

*Restrictions on the complexity of the problem*
Since the size of arrays depends strongly on the nuclear shell and the number of particles, provision is made for easy adjustment of dimensions. However, the number of components of a highest weight state in the many-particle basis should not exceed 200 or else truncation error may accumulate.

*Typical running time*
It is a critical function of the nuclear shell, the number of particles, as well as the options selected.

*Unusual features of the program*
All the large integer arrays which store numbers that are always less than 256 start with the letter "L". Therefore in IBM 360/370 or similar operating systems advantage may be taken of the statement IMPLICIT INTEGER*2(L) to save up to 35% of high speed storage.

*References*

[1] Y. Akiyama and J.P. Draayer, Comp. Phys. Comm. 5 (1973) 405.
[2] K.T. Hecht and D. Braunschweig, Nucl. Phys. A244 (1975) 365.

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* Work supported by the U.S. National Science Foundation.

** Block 3 of the program was developed at The Weizmann Institute, Rehovot, Israel.

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# CALCULATION OF WAVE–FUNCTIONS AND COLLISION MATRIX ELEMENTS FOR ONE-ELECTRON DIATOMIC MOLECULES

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Received 10 October 1977

## PROGRAM SUMMARY

*Title of program*: GRAVE

*Catalogue number*: ACXX

*Computer*: IRIS 80; *Installation:* Centre de Calcul Interuniversitaire, Bordeaux, France

*Operating system*: SIRIS 8

*Programming language used*: FORTRAN

*High speed storage required*: 12 K words

*No. of bits in a word*: 32

*Overlay structure*: optionally overlaid

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer and preferably magnetic disks.

*No. of cards in combined program and test deck*: 692

*Keywords*: Atomic physics, collision, diatomic, molecule, one-electron, ion-atom, wave function, bound state

*Nature of the physical problem*
Determination of the wave-functions for one-electron diatomic molecules by semi-analytic expansions. Results may be used by the program MEDØC to calculate collision matrix elements.

*Method of solution*
The problem is reduced to the solution of a system of linear equations. The method used is that of Martin and Wilkinson [1].

*Restrictions on the complexity of the problem*
The eigen-energies should be obtained beforehand (a very efficient program is available [2]). Bound states only.

*References*

[1] R.S. Martin and J.H. Wilkinson, Contribution I/6 in: Handbook for Automatic Computation, vol. II, J.H. Wilkinson and C. Reinsch eds. (Springer-Verlag, Berlin, 1971).
[2] J.D. Power, QCPE Program 233, Quantum Chemistry Program Exchange, Chemistry Department, Indiana University, U.S.A.

## PROGRAM SUMMARY

*Title of program*: MEDØC

*Catalogue number*: ACXY

*Computer*: IRIS 80; *Installation*: Centre de Calcul Interuniversitaire, Bordeaux, France

*Operating system*: SIRIS 8

*Programming language used*: FORTRAN

*High speed storage required*: 14 K words

*No. of bits in a word*: 32

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* Equipe de Recherche du CNRS N° 137.

*Overlay structure*: Optionally overlaid

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer and preferably magnetic disks.

*No of cards in combined program and test deck*: 1120

*CPC Library programs used*: *Cat. no.*: ACXX; *Title*: GRAVE; *Ref. in CPC*: this paper.

*Keywords*: atomic physics, collision, ion-atom, diatomic, one-electron, molecule, collision matrix element, bound state

*Nature of the physical problem*: Determination of the norm of the wave-functions and of radial and rotational coupling matrix elements between the states of one electron diatomic molecules. The wave-functions are given by the program GRAVE.

*Method of solution*

The integrations are carried out either analytically or by Gauss–Laguerre quadratures.

*Restriction on the complexity of the problem*

Bound states only.

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# DWBA PROGRAM FOR HEAVY ION TRANSFER REACTIONS

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Received 24 October 1977

## PROGRAM SUMMARY

*Title of program*: DAISY

*Catalogue number*: ABMY

*Computer*: CDC 7600; *Installation*: University of Manchester Regional Computing Centre

*Operating system*: UMRCC Scope V2.1

*Programming language used*: FORTRAN

*High speed storage required*: 40 K words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1926

*Keywords*: nuclear, heavy ion, DWBA, finite range, transfer reaction, cross section, low energy, scattering

*Nature of physical problem*
The program calculates the differential and integrated cross section for the transfer of nucleons or $\alpha$-particles in heavy ion reactions. The Finite range Distorted Wave Born approximation [1] is used, and all nuclear and Coulomb terms in the interaction are retained.

*Method of solution*
The six-dimensional DWBA integral is reduced by standard angular momentum theory to a sum of three-dimensional integrals. These are done numerically using Gaussian quadrature. An attempt has been made to reduce the input data as far as is reasonable, so that users who are not familiar with the programme can run it reliably. Both post and prior formalisms are possible and agreement between the two can be obtained to within 1%.

*Restrictions on the complexity of the problem*
The program deals only with one step transfer of spin $\frac{1}{2}$ or spin zero particles. It does not allow for spin orbit forces in the distorted waves. It is restricted to 124 partial waves, although this limit could easily be increased.
The maximum bound state orbital angular momentum is $l = 8$.

*Typical running time*
For light projectiles and targets, such as $^{12}C$ or $^{16}O$, with low angular momentum transfer, runs of about 12 s are needed on the CDC 7600. For heavy targets such as lead, with high angular momentum transfer, run times increase to about 3 min. All possible angular momentum transfers are included in a single run. The test run $^{26}Mg(^{16}O, ^{15}N)^{27}Al$ at 45 MeV took 23 s on the CDC 7600 and 3 min on the IBM 370/165.

*References*

[1] W. Tobocman, Theory of Direct Nuclear Reactions (Oxford, 1961).

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# A GENERAL MULTI-CONFIGURATION HARTREE–FOCK PROGRAM

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*Department of Computer Science, The Pennsylvania State University, University Park, PA 16802, USA*

Received 8 November 1977

## PROGRAM SUMMARY

*Title of program*: MCHF77

*Catalogue number*: ACYA

*Computer*: IBM S370/168; *Installation*: The Pennsylvania State University, University Park, PA

*Operating system*: OS/MVT Release 21-8

*Programming language used*: FORTRAN IV

*High speed store required*: 69k words.

*No. of bits in a word*: 32

*Overlay structure:* none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader; punch; printer

*No. of cards in combined program and test deck*: 4414

*Reference to other published version of this program*:

| *Cat. No.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACQJ | MULTI-CONFIGURATION HARTREE–FOCK | 1 (1969) 151 |
| ACRF | MCHF72 | 4 (1972) 107 |

*Keywords*:
atomic structure, numerical Hartree–Fock, configuration interaction, bound state, Schrödinger equation, wavefunction, self-consistent field, energy level.

*Nature of physical problem*
Numerical non-relativistic Hartree–Fock results are determined within the multi-configuration approximation for atoms in a bound state.

*Method of solution*
The self-consistent field method of solution is employed. In a multi-configuration calculation the mixing coefficients are adjusted periodically as part of the SCF iteration. Two methods of solution of the differential equations are used, each improving only a single function at a time [1], and rotations are introduced explicitly to find on energy stationary with respect to a rotation of the orbital basis. Otherwise the procedures are essentially the same as those in MCHF72 [2].

*Restrictions on the complexity of the problem*
The possible configuratiins are restricted to those for which the interactions can be expressed as either $F^k$, $G^k$, $R^k$ or $I_{nl,n'l}$ integrals. Configurations differing by one electron may be included provided that the resulting MCHF problem has a unique solution [3]. Since bound states in the continuum interact most strongly with continuum states, a multi-configuration calculation for such states cannot be performed with this program.

*Unusual features of the program*
The organization of the program is such that the "frozen core" approximation may be used and orbitals with zero occupation number are allowed. Orbitals in different configurations may be allowed to differ so long as not more than one overlap integral enters into the expression for the interaction and the expressions for off-diagonal energy parameters remain relatively simple. A fixed zero-order approximation may be employed resulting in a considerable saving in computation time in some cases.

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* Supported in part by the U.S. Energy Research and Development Administration.

*References*

[1] C. Froese Fischer, J. Comput. Phys. 15 (1977) to appear.
[2] C. Froese Fischer, Computer Phys. Commun. 4 (1972) 107
[3] C. Froese Fischer, J. Phys. B.3 (1970) 779.

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# I. A COMPUTER PROGRAM FOR GENERATION OF A COMPLETE SET OF COORDINATES AND FORCE MATRICES FOR NORMAL MODE CALCULATIONS OF CRYSTALS AND MOLECULES

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Received 12 January 1977
Revised manuscript received 12 December 1977

## PROGRAM SUMMARY

*Title of program*: FYCOOR

*Catalogue number*: ACXQ

*Computer*: IBM 370/165; *Installation*: NEUCC, The Technical University of Denmark.

*Operating System*: OS/MVT, Release 21.7

*Programming language used*: FORTRAN IV

*High speed storage required*: 48500 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, magnetic disc (6 files)

*No. of cards in combined program and test deck*: 1682

**CPC Library subprograms used**

| *Cat. No.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACXR | FYFRE | This issue |
| ACXS | FYADJ | This issue |

*Keywords*: solid state physics, crystal, molecule, normal mode, coordinate, force constant, group theory, symmetry.

*Nature of physical problem*
In this paper we describe a computer code, FYCOOR, for generation of a complete set of coordinates to be used in a normal mode calculation for crystals or for molecules. This program eliminates or reduces time-consuming and error producing complexities, which have handicapped the application of some computer programs for calculating normal modes.

*Method of solution*
Group theory is used in the program in such a way, that many (often most) of the coordinates used for the potential energy are generated from a minimum input of "basis-set coordinates", which may be arbitrary. All force constant matrices are set up by the program with very small "dummy" force constants that are easily updated in a selective manner by the user to give the desired potential. The program includes a logic, which assures that force constants, which are interrelated by symmetry are correctly displayed and used, and there are provisions, which check if the potential is invariant against pure rotations and translations.

*Typical running time*
The running time depends on the problem. In the case of diamond, where the number of symmetry operations is 48, the running time for 2 input coordinates with 4 interaction types was 120 s. In the case of selenium, where the number of symmetry operations is 6, the running time for 3 input coordinates with two interaction types was 20.6 s, and for 9 input coordinates with one interaction type it was 33.6 s. The compilation time of 12.2 s is included in these times.

*Restrictions on the complexity of the problem*
In the present version 20 input coordinates, 10 atoms per unit cell or per molecule, 10 interaction types and 48 symmetry operations (which are the maximum number of operations to occur) may be considered. Detailed information on how to alter the present dimensions may be found in the long write-up.

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# II. A PROGRAM FOR COMPUTING NORMAL MODES OF MOLECULES, CRYSTAL PHONON DISPERSION RELATIONS AND STRUCTURE FACTORS FOR NEUTRON INELASTIC SCATTERING

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Received 21 July 1977
Revised manuscript received 12 December 1977

## PROGRAM SUMMARY

*Title of program*: FYFRE

*Catalogue number*: ACXR

*Computer*: IBM 370/165 *Installation*: NEUCC, The Technical University of Denmark

*Operating system*: OS/MVT, Release 21.7

*Programming language used*: FORTRAN IV

*High speed storage required*: 57500 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, magnetic disc (6 files)

*No. of cards in combined program and test deck*: 1284

**CPC Library subprograms used**

| *Cat. No* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACXQ | FYCOOR | This issue |
| ACXS | FYADJ | This issue |

*Keywords*: solid state physics, crystal, molecule, normal mode, neutron, structure factor, dispersion relation, group theory, symmetry, dynamical matrix, phonon, annihilation, creation

*Nature of physical problem*
The calculation of normal modes in molecules and crystals based on a harmonic potential field defined in terms of any set of coordinates. For crystals the structure factors and partial differential cross sections for inelastic one phonon annihilation processes and one phonon creation processes are calculated taking temperature effects into account. Also, the polarization factors for each atom in the unit cell is calculated for each normal mode.

*Method of solution*
The calculations are based on the results of program FYCOOR described in part I, which generates a complete set of coordinates and force matrices from a very limited input of basis coordinates. These results are stored on permanent units and used in the present program, which calculates the dynamical matrix by simple matrix operations. Symmetry coordinate matrices are used to block diagonalize the dynamical matrix. Once the normal frequencies and eigenvectors have been calculated the inelastic one phonon structure factors and related quantities are calculated.

*Typical running time*
The running time depends on the problem. For the two test runs the running times including the compilation time were 16 s and 18 s. The compilation time is 12 s.

*Unusual features of the program*
The storage requirement depends on the problem that is the number of atoms in the unit cell or in the molecule, the number of basis coordinates and the number of updated force constants. In the present set up the storage requirement is set to 57500 words, which is estimated to be sufficient for

a number of cases. Up to 20 basis coordinates, 10 atoms per unit cell or per molecule and 30 updates of force constants may be considered. For a more precise estimate of the storage requirement one should consult the long write up. Detailed information on how to change storage requirements may also be found there.

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# III. A FORCE CONSTANT ADJUSTER PROGRAM TO OBTAIN LEAST SQUARES FIT TO OBSERVED FREQUENCIES OF MOLECULES AND CRYSTALS

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Received 21 July 1977
Revised manuscript received 12 December 1977

## PROGRAM SUMMARY

*Title of program*: FYADJ

*Catalogue number*: ACXS

*Computer*: IBM 370/165 *Installation*: NEUCC, The Technical University of Denmark

*Operating System*: OS/MVT, Release 21.7

*Program language used*: FORTRAN IV

*High speed storage required*: 47500 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, magnetic disc (2 files)

*No. of cards in combined program and test deck*: 848

**CPC Library subprograms used:**

| *Cat. No.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACXQ | FYCOOR | This issue |
| ACXR | FYFRE | This issue |

*Nature of physical problem*
The objective of the present program is to determine the values of a given set of force constants for the internal vibration of molecules or crystals in the harmonic approximation, in such a way as to give a least squares fit of calculated frequencies to observed frequencies.

*Method of solution*
The calculations with this program are based on the results of the FYFRE program described in part II, where data for the generation of the analytic form of the dynamical matrix in terms of relevant force constants have been obtained. The eigenvalues of the Hermitian matrix, which has been blocked diagonalized by symmetry coordinate matrices, are calculated and compared with observed frequencies. An iterative determination of the force constants are performed using a procedure, where only the calculated frequencies need to be entered, while derivatives of the frequencies with respect to force constants do not have to be entered.

*Typical running time*
The running time obviously depends in particular on the number of iterations to be performed and to a lesser degree on the nature of the problem. For the test example considered here the running time for 10 iterations were 12 s including compilation time. The compilation time for the program is 7 s.

*Unusual features of the program*
The storage requirement depends on the problem, that is the number of normal modes, and the number of non zero elements of the dynamical matrix. In the present set up the storage requirement is set to 47500 words. Problems with up to 30 normal modes and 500 non zero matrix elements may be considered, while up to 10 force constants may be determined simultaneously in one calculation and up to 100 experimental frequencies may be considered. One should consult the long write up for details.

*Restrictions on the complexity of the problem*
The only restriction of the program is the high speed storage available.

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# EXACT SLATER INTEGRALS

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Received 21 April 1977

## PROGRAM SUMMARY

*Title of program*: SLATER INTEGRALS

*Catalogue number*: ACYB

*Computer*: IBM 370/168; *Installation*: The Pennsylvania State University, University Park, Pa. 16802 USA

*Operating system*: IBM OS-21.8, HASP – 2.T4E

*Programming language used*: PL/1-FORMAC

*High speed storage required*: 1027 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 188

*Keywords*: Atomic Physics, Structure, Slater intergrals, non-numeric, hydrogenic, wave function.

*Nature of physical problem*
In atomic structure calculations, one has to evaluate the Slater integrals [1]. In the present program, we evaluate exactly the Slater integral when hydrogenic wave functions are used for the bound-state orbitals.

*Method of solution*
When hydrogenic wave functions are used, the Slater integrals involve integrands which can be written in the form of a product of an exponential, exp($ax$) and a known analytic polynomial function, f($x$). By repeated partial integration such an integral can be expressed in terms of a finite series involving the exponential, the polynomial function and its derivatives. PL/1-FORMAC has a built-in subroutine that will analytically find the derivatives of any multinomial [2,3]. Thus, the finite series and hence the Slater integral can be evaluated analytically.

*Restrictions on the complexity of the problem*
FORMAC square roots should be in the form

ROOT. (NUMBER) .

The function, f($x$), must be of order 20 or less. The order can be increased by increasing the upper limit on each occurrence of the DO function in the program. There must be no numbering or ID data on the data cards.

*Typical running time*
The running times for the test run are as follows:

Compile time – 2 s, CPU time – 5 s,
Elapsed time – 12 s.

*Unusual features of the program*
This program is a non-numeric routine. It evaluates the Slater integral analytically. The results are exact.

*References*

[1] E.U. Condon and G.H. Shortley, The Theory of Atomic Spectra, (Cambridge University Press, London, 1951).
[2] K.A. Bahr, Share 45 Proceedings, (Share, Inc., 1975).
[3] K.A. Bahr, Sigsam Bull. 9 (1975) 21.

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Computer Physics Communications 14 (1978) 261–265
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# SPHERICAL BESSEL FUNCTIONS $j_n$ AND $y_n$ OF INTEGER ORDER AND REAL ARGUMENT

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Received 8 October 1976
Revised manuscript received 8 December 1977

## PROGRAM SUMMARY

*Title of program*: SPHBES

*Catalogue number*: ACXM

| *Computer*: | *Installation*: |
|---|---|
| CDC 6600 | University of London Computer Centre |

*Operating system*: CDC Scope

*Programming language used*: FORTRAN IV

*High speed storage required*: 3 K words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 558

*Keywords*: General purpose, atomic, nuclear, acoustic, scattering, phase shift, radial, partial wave, spherical Bessel functions

*Nature of the physical problem*

The spherical Bessel function appears in a variety of physical applications, and especially in phase shift analysis. The package SPHBES contains a subroutine to calculate $j_n(x)$ and $y_n(x)$ for any integer order $n$ and real argument $x$. The functions $j_n(x)$ and $y_n(x)$ are produced simultaneously and efficiently.

*Method of solution*

The spherical Bessel functions are generated using formulae given in [1].

*Restrictions on the complexity of the problem*

The results are dependent on the size of the real number that can be accommodated by the computer. Due to partial cancellation of large numbers, precision is lost when both a large argument and a large order are involved.

*Typical running time*

The test run output took about 0.6 seconds.

*References*

[1] M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables (Dover Publications, Inc., New York, 1965).

Computer Physics Communications 14 (1978) 267–272
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# INNER MULTIPLICITY OF UNITARY GROUPS

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and

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Received 15 June 1977
Revised manuscript received 12 December 1977

## PROGRAM SUMMARY

*Title of program*: IMUG

*Catalogue number*: AAAJ

*Computer*: PDP-11/50; *Installation*: Dept. of Computer Science, U.W.O., London

*Operating system*: RSTS/E

*Program language used*: BASIC-PLUS [1]

*High speed storage required*: 4K words

*No. of bits in a word*: 16

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: disk and terminal

*No. of cards in combined program and test deck*: 353

*Keywords*: general purpose, Lie algebra, inner multiplicity, unitary groups, Gelfand patterns

*Nature of the problem*
To compute the inner multiplicity of a particular weight in a given representation for the special unitary groups using Gelfand patterns.

*Method of solution*
There exists a rather simple method of calculating the inner multiplicity of weights of $SU(n)$ by means of Gelfand patterns. The method of solution is given by Gruber and Delaney [2] in their paper on classical groups and consists of counting all distinct Gelfand patterns which belong to the same weight.

*Restriction on the complexity of the problem*
The program handles $SU(n)$ groups with rank less than or equal to 9.

*Typical running time*:
The multiplicity $\gamma(1,0,0,0,0,-1) = 5$ in the representation $D(2,0,0,0,0,-2)$ is calculated in 3.6 s. The multiplicity $\gamma(0,0,0,0,0,0,0,0,0,0) = 90$ in the representation $D(1,1,1,1,0,0,-1,-1,-1,-1)$ is calculated in 30.9 s.

*Unusual features of the program*
Since the multiplicity of a particular weight in an irreducible representation is calculated without any references to other weights except the highest weight there is no restriction on the dimension of the representation. The program of Kolman and Beck [3] is restricted in the dimension (fewer than 1000 weights). The program can also be used to obtain the various possible Gelfand patterns from a given partition.

*References*

[1] Basic-Plus Language Manual (Order No. DEC-11-ORBPA-B-D1) Digital Equipment Corporation, Software Distribution Center, Maynard, Massachusetts 01754, USA.
[2] R.M. Delaney and B. Gruber (J. Math. Phys. 10 (1969) 252.
[3] B. Kolman and R.E. Beck, Comput. Phys. Commun. 6 (1973) 24.

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Computer Physics Communications 14 (1978) 273–285
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# INTER-ELECTRON REPULSION INTEGRALS FOR THREE-OPEN-SHELL CONFIGURATIONS IN CUBIC SYMMETRY

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Received 14 March 1977

## PROGRAM SUMMARY

*Title of program*: TRIO

*Catalogue number*: AAKT

*Computer*: IBM 370–145; *Installation*: Centre de Calcul de Fribourg, La Chassotte, CH-1700 Fribourg

*Operating system*: OS/VS1 R 06.0

*Programming language used*: FORTRAN IV

*High speed storage required*: 140 Kbytes

*No. of bits in a byte*: 8

*Overlay structure*: None

*No. of magnetic tapes required*: None

*Other peripherals used*: Card reader, line printer, disk space

*No. of cards in combined program and test deck*: 2186

*Keywords*: Molecular physics, quantum chemistry, theoretical method, electrostatic repulsion, integrals, irreducible tensor method, Racah $\overline{V}$, $\overline{W}$ and $\overline{X}$ coefficients, [**] fractional parentage coefficient, Wigner–Eckart theorem, reduced matrix elements

*Nature of the physical problem*
Molecules of high symmetry containing incompletely filled electronic shells, such as transition metal complexes, have excited states whose energies are determined by differences in one-electron orbital energies and changes in electron repulsion energy as the electrons are rearranged on going from the ground to the excited states. This program calculates the contribution of electron repulsion to the energies of electronic-states containing three open shells. It is especially useful for charge transfer configurations [1].

*Method of solution*
The vector coupling technique [2,3] is used to express the repulsion integrals in the strong field scheme as a linear combination of reduced matrix elements which can not be further reduced by symmetry.

*Restriction on the complexity of the problem*
Only shells with different symmetries can be calculated, except for those spanning the irreducible representation $t_2(\Gamma_5)$, in which case two shells may have the same symmetry.

*Typical running time*
42 s compilation time, 0.5 s for diagonals and 0.1 for non-diagonal matrix elements.

*References*
[1] B. Bird et al., Phil. Trans. Royal Soc. London 276 (1974) 277.
C. Daul and P. Day, Mol. Phys. 33 (1977) 1421.
[2] J.S. Griffith, The Irreducible Tensor Method for Molecular Symmetry Groups (Prentice-Hall International, London, 1962).
[3] J.S. Griffith, The Theory of Transition Metal Ions (Cambridge at the University Press, 1971).

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[*] Permanent address: Institut de Chimie Inorganique, Université de Fribourg, 1700 Fribourg, Switzerland, and to whom correspondence should be addressed.

[**] Griffith $V$, $W$ and $X$ coefficients.

Computer Physics Communications 14 (1978) 287–297
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# SIMULATION OF THE GROWTH OF AXIALLY SYMMETRIC DISCHARGES BETWEEN PLANE PARALLEL ELECTRODES

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Received 13 December 1977

## PROGRAM SUMMARY

*Title of program*: SPARK2

*Catalogue number*: ABUU

*Computer*: CDC 7600; *Installation*: Manchester Regional Computer Centre

*Operating system*: Scope

*Programming language used*: FORTRAN

*High speed storage required*: 87000 words

*No. of bits in a word*: 60

*Overlay structure*: None

*No. of magnetic tapes required*: 2 at most

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 2253

*Reference to other published versions of this program*:

*Cat. no:* ABUD; *Title*: SPARK 71; *Ref. in CPC*: 3 (1972) 322

*Keywords*: Plasma, atomic, electrical discharge, electrical breakdown, space-charge, plane-parallel electrodes, positive ion, negative ion, electron, photon, cathode

*Nature of physical problem*
SPARK2 computes the axial and radial development of an axially symmetric electrical discharge between plane parallel electrodes. The processes incorporated are primary ionization, attachment, detachment, secondary cathode emission due to the incidence of photons and positive ions, space-charge distortion of the applied field and the properties of the external electrical circuit. SPARK2 is a two-dimensional extension of SPARK71 [1]. It is complementary to and not a replacement for this program.

*Method of solution*
The charge densities of the electrons and negative ions, and the net charge density, are governed by time-dependent hyperbolic differential equations in two space dimensions. The equations for the electrons and negative ions are integrated along the two characteristic directions in $(x, r, t)$ space, while the equation for the net density is solved by an implicit finite difference scheme. Iteration in the $t$-direction allows the change in the coefficients of the equations, due to field distortion, to be followed. The electric potential is found by solving Poisson's equation by the fast Fourier transform technique. The $x$-axis is divided into equal meshes but the mesh points on the $r$-axis can be chosen arbitrarily.

*Restrictions on the complexity of the problem*
As given in the listing, the program will accommodate up to 64 meshes in the $x$-direction, with 20 meshes in the $r$-direction for the density calculation and 40 meshes in the $r$-direction for the potential calculation. These numbers may be increased by changing the DIMENSION and COMMON statements.

*Unusual features of the program*
When a certain stage in the discharge development has been reached the non-linearity of the equations becomes so strong that an impossibly high order of accuracy is needed to ensure convergence, and the program will eventually fail due either to instability leading to overflow or to the time step becoming too small for any progress to be made.

*References*

[1] A.J. Davies and C.J. Evans, Computer Phys. Commun. 3 (1972) 322.

Computer Physics Communications 14 (1978) 299–309
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# A NUMERICAL CALCULATION OF MULTIDIMENSIONAL INTEGRALS

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*Institute of Physics, Technical University of Warsaw, Koszykowa 23, PL-00-662 Warsaw, Poland*

Received 10 June 1977
Revised manuscript received 25 January 1978

## PROGRAM SUMMARY

*Title of program*: KOROBO

*Catalogue number*: ACXU

*Computer*: CDC 6400; *Installation*: Computing Centre of the Institute for Nuclear Research, Warsaw, Poland

*Operating system*: SCOPE

*Program language used*: FORTRAN IV

*High speed storage required*: 20723 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 430

*Keywords*: general purpose, numerical integration, multiple integrals, Korobov method

*Nature of the physical problem*:
Calculation of the multidimensional integrals of quantum mechanics, quantum chemistry, nuclear physics, solid state physics, etc.; for example, calculation of the single particle overlap integrals, matrix elements of the single particle hamiltonian (e.g. Coulomb interaction potentials).

*Method of solution*
The method is based on the number theory approach described in detail in [1]. The multidimensional integrals are approximated by finite sums of the function values calculated for a specially optimized lattice.

*Restriction of the complexity of the problem*
The program can be applied to integration of functions of $s \geqslant 2$ variables. It is assumed that the function is integrable in the specified integration area.

*Typical running time*
The running time depends strongly on the complexity of the function to be integrated and on the declared number, $N$, of grid points of the lattice.

*References*

[1] N.M. Korobov, The Number Theory Methods in the Approximation Analysis (in Russian) (Gos. Izdat. Faz.-Mat. Lit., Moscow, 1963).

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# ERRATUM NOTICE

*Title of manuscript*: CFPJJ – Fractional parentage coefficients for equivalent electrons in *jj*-coupling

*Author*: I.P. Grant

*Reference*: Comput. Phys. Commun. 4 (1972) 377

*Title of program*: CFPJJ

*Catalogue number*: ACRI

*Title of manuscript*: A program to calculate angular momentum integrals in relativistic atomic structure – revised version

*Author*: I.P. Grant

*Reference*: Comput. Phys. Commun. 11 (1976) 397

*Title of program*: MCP75

*Catalogue number*: ACWE

Computer Physics Communications 14 (1978) 327–365
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# BNDPKG. A PACKAGE OF PROGRAMS FOR THE CALCULATION OF ELECTRONIC ENERGY BANDS BY THE LCGO METHOD *

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Received 16 August 1977

## PROGRAM SUMMARY

*Title of program*: BNDPKG

*Catalogue number*: ACXZ

*Computer*: IBM 360/65; *Installation*: Systems Network Computer Centre Louisiana State University, Baton Range, Louisiana 70803, USA

*Operating system*: OS/360

*Program language used*: FORTRAN IV

*High speed storage required*: words 238 000 bytes + 176 000 bytes extended.

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, scratch disc, permanent disc

*No. of cards in combined program and test deck*: 8373

*Keywords*: solid state physics, crystal, band structure, Bloch function, self-consistent, density of states, LCGO method

*Nature of physical problem*
This program calculates self-consistent energy levels, wave functions, and the density of states for cubic crystals with one atom per unit cell (simple cubic, body centered, or face centered) by expansion in a set independent Gaussian orbitals.

*Method of solution*
(i) A starting potential is constructed from overlapping atomic charge densities. Fourier coefficients of this potential are determined.
(ii) Hamiltonian, overlap, and generalized overlap integrals are computed using a basis of independent Gaussian orbitals. The integrals are performed analytically. The basis set is tested for approximate linear dependence.
(iii) The Hamiltonian and overlap matrices are diagonalized to obtain energy levels and wave functions for the starting potential.
(iv) Wave functions from step (iii) are used to construct the change in the charge density and in the potentials. The starting potential is modified, and the process is repeated until convergence is obtained.
(v) After convergence of the self-consistent procedure, final final corrections are made to the potential. The Hamiltonian integrals are recalculated. Final energy bands and the density of states are determined.

*Restrictions on the complexity of the problem*
The program is specifically limited to simple, body centered, and face centered cubic crystals. Ferromagnetic (but not anti-ferromagnetic) order is allowed.

Practical considerations limit the application of the program to atoms of large atomic number. Although integrals can be calculated for s, p, d, and f orbitals, the number of Gaussian functions required to give a good description of atomic wave functions in heavy atoms increases. We have made band calculations for atoms as heavy as nickel; the

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heaviest atom for which analytic self-consistent field wave functions required in the construction of the starting charge density are available at present is zinc. The dimensions of variables are appropriate for the test case of this program (for which data is also given), which is the band structure of body centered cubic lithium. Dimensions will have to be altered for other cases. Comments concerning dimensioning of variables will be found elsewhere in the text.

*Typical running time*
Execution time depends primarily on the number of Gaussian orbitals included in the basic set, and the number of iterations required to achieve self-consistency. Approximately twice as much time will be required if ferromagnetic order is considered.

The test case for which data is included in the package, the band structure of lithium, requires a total of 89 min on an IBM 360/65.

*Unusual features of the program*
The program is written in IBM 360 extended FORTRAN. Non-standard features include:

(1) Arrays with more than three dimensions.
(2) Apostrophes to define hollerith strings in Format and Data statements.
(3) Data set in type statements.
(4) Array element expressions involving more than one variable.
(5) READ statements including end-of-data jump, e.g. READ(1, END = 210)
(6) IMPLICIT statements.

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# A NEW VERSION OF THE GENERAL PROGRAM TO CALCULATE ATOMIC CONTINUUM PROCESSES USING THE R-MATRIX METHOD

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K.T. TAYLOR ☆ and Vo Ky LAN **

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*** Group T4, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, USA
☆ Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, Colorado 80309, USA

Received 6 December 1977

## PROGRAM SUMMAY

*Title of program*: A NEW VERSION OF RMATRX STG1

*Catalogue number*: AAHF

*Computer*: IBM 360/195; *Installation*: Rutherford Laboratory, Chilton, Didcot, Oxfordshire, England

*Operating system*: OS/360 MVT-HASP

*Programming language used*: FORTRAN IV

*High speed storage used*: 522 000 bytes.

*No of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: 1

*Other peripherals used*: card reader, line printer, scratch disc store, permanent disc store

*No. of cards in combined program and test deck*: 5119

*Reference to other published version of this program*:

| *Catalogue number*: | *Title*: | *Ref. in CPC*: |
|---|---|---|
| AAHA | RMATRX STG1 | 8 (1974) 149 |

*CPC Library subprograms used*:

| *Catal. number* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAHG | A NEW VERSION OF RMATRX STG2 | This paper |
| AAHH | A NEW VERSION OF RMATRX STG3 | This paper |

*Keywords*: Atomic, electron–atom, scattering, electron–ion, photo-ionization, polarizability, *R*-matrix, continuum, bound, pseudo-potential, de Vogelaere's method, radial integrals, RK integrals.

*Nature of the physical problem*
This program calculates all one-electron, two-electron and multipole radial integrals involving bound and continuum orbitals. These radial integrals enable electron–atom or electron–ion scattering, photoionization or frequency dependent polarizabilities to be calculated for a general atomic system [1]. The bound orbitals are specified analytically. The continuum orbitals are calculated by the program. The integrals are stored on a magnetic tape or disc file for use by A NEW VERSION of RMATRX STG2 [2].

*Method of solution*
The continuum orbitals are determined by integrating numerically a differential equation with a given potential using de Vogelaere's method and subject to *R*-matrix boundary conditions. The radial integrals are evaluated numerically using Simpson's rule.

*Restrictions on the complexity of the program*
Up to 5 bound orbitals and 20 continuum orbitals can be included for each angular momentum up to $l = 14$. More orbitals can be included by recompiling with larger dimensions; in this case, certain arrays which contain the radial integrals may have to have their dimensions increased for large runs.

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*Typical running time*
The running time depends approximately on the square of the number of bound orbitals, on the square of the number of continuum orbitals for each angular momentum, and on the number of continuum angular momenta. The test run took 53 s on the IBM 360/195.

*References*

[1] P.G. Burke and W.D. Robb, in: Advances in Atomic and Molecular Physics, vol. 11, D.R. Bates and B. Bederson, eds. (Academic Press, New York, 1975) p. 143.

[2] K.A. Berrington, P.G. Burke, M. le Dourneuf, W.D. Robb, K.T. Taylor and Vo Ky Lan (this paper).

## PROGRAM SUMMARY

*Title of program*: A NEW VERSION OF RMATRX STG2

*Catalogue number*: AAHG

*Computer*: IBM 360/195; *Installation*: Rutherford Laboratory, Chilton, Didcot, Oxfordshire, England

*Operating system*: OS/360 MVT-HASP

*Programming language used*: FORTRAN IV

*High speed storage required*: 628 000 bytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: 3

*Other peripherals used*: card reader, line printer, scratch disc store, permanent disc store

*No. of cards in combined program and test deck*: 10154

*Reference to other published version of this program*:

| *Catalogue number*: | *Title*: | *Ref. in CPC*: |
|---|---|---|
| AAHB | RMATRX STG2 | 8 (1974) 149 |

*CPC Library subprograms used*:

| *Catal. number* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAHF | A NEW VERSION OF RMATRX STG1 | This paper |
| AAHH | A NEW VERSION OF RMATRX STG3 | This paper |

*Keywords*: atomic, electron–atom, scattering, electron–ion, photoionization, polarizability, *R*-matrix, hamiltonian matrix, ionic, Racah coefficient, fractional parentage coefficient, recoupling, angular integral, continuum, bound, LS coupling, long-range potentials, dipole matrix elements.

*Nature of the physical problem*
This program reads the radial integrals stored on a magnetic tape or disc file by A NEW VERSION OF RMATRX STG1 [1]. It then calculates the hamiltonian matrix elements, the asymptotic potential coefficients, and the dipole length and velocity matrix elements from a given initial state to the final state specified by L, S and the channel quantum numbers. These quantities are stored on a magnetic tape or disc file for use by A NEW VERSION OF RMATRX STG3 [1].

*Method of solution*
The triangular relations are used to determine the number of coupled channels given the value of L and S and the quantum numbers of the atomic states. The angular integrals are carried out using the methods of Racah algebra. These are then combined with the radial integrals evaluated by A NEW VERSION OF RMATRX STG1.

*Restrictions on the complexity of the program*
Up to 20 continuum orbitals can be included for each angular momentum up to $l = 14$. This number can be increased by recompiling with larger dimensions. The program assumes that L and S are good quantum numbers and neglects effects due to the spin-orbit interaction.

*Typical running time*
The running time depends on the square of the number of shells and the number of configurations included. The test run took 6 s on the IBM 360/195.

*References*

[1] K.A. Berrington, P.G. Burke, M. le Dourneuf, W.D. Robb, K.T. Taylor and Vo Ky Lan (this paper).

## PROGRAM SUMMARY

*Title of program*: A NEW VERSION OF RMATRX STG3

*Catalogue number*: AAHH

*Computer*: IBM 360/195; *Installation*: Rutherford Laboratory, Chilton, Didcot, Oxfordshire, England

*Operating system*: OS/360 MVT-HASP

*Programming language used*: FORTRAN IV

*High speed storage used*: 654 000

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: 2

*Other peripherals used*: card reader, line printer, scratch disc store, permanent disc store

*No. of cards in combined program and test deck*: 7244

*Reference to other published version of this program*:

| *Catalogue number*: | *Title*: | *Ref. in CPC*: |
|---|---|---|
| AAHC | RMATRX STG3 | 8 (1974) 149 |

*CPC Library subprogram used*:

| *Catal number* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAHF | A NEW VERSION OF RMATRX STG1 | This paper |
| AAHG | A NEW VERSION OF RMATRX STG2 | This paper |

*Keywords*: atomic, electron–atom, scattering, electron-ion, photoionization, polarizability, $R$-matrix, hamiltonian matrix, Householder method, eigenvalues, eigenvectors, cross sections, Buttle correction, De Vogelaere's method, phase shifts, $K$-matrix, $T$-matrix, long-range potentials, asymptotic solutions, WBK.

*Nature of the physical problem*

This program reads the hamiltonian matrix elements, the asymptotic potential coefficients and the dipole length and velocity matrix elements stored on a magnetic tape or disc file by A NEW VERSION OF RMATRX STG2 [1]. It then diagonalizes the hamiltonian matrix and calculates the $R$-matrix and its Buttle correction. Then either the electron–atom or electron–ion cross section, the photoionization cross section and $\beta$ asymmetry parameter or the frequency dependent polarizability is calculated, for a range of incident energies or frequencies. In a photoionization or polarizability calculation, the initial state is treated in exactly the same way as the final states.

*Method of solution*

The Householder method and the bisection method are used to diagonalize the hamiltonian matrix, and the Buttle correction to the $R$-matrix is calculated by solving a differential equation using the Vogelaere's method. In the case of electron scattering and photoionization, the coupled differential equations are solved in the asymptotic region using either an asymptotic series expansion or a WBK solution. The $K$-matrix and $T$-matrix are determined from the $R$-matrix by matrix algebra.

*Restrictions on the complexity of the program*

The maximum size of the hamiltonian matrix that can be treated is 200, the maximum number of channels is 12 and the maximum number of energies which can be dealt with in one run is 50. All of these can be increased by recompiling with larger dimensions.

*Typical running time*

For most practical runs, the time taken to solve the coupled differential equations in the asymptotic region is usually the dominating factor. The test run took 3 s for electron scattering, 6 s for photoionization and 6 s for polarizability on the IBM 360/195.

*References*

[1] K.A. Berrington, P.G. Burke, M. le Dourneuf, W.D. Robb, K.T. Taylor and Vo Ky Lan (this paper).

Computer Physics Communications 14 (1978) 413–421
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# WEIGHT MULTIPLICITY FOR UNITARY GROUPS

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*Istituto Nazionale di Fisica Nucleare, Sezione di Milano, Italy*

Received 22 June 1977; in revised form 25 January 1978

## PROGRAM SUMMARY

*Title of programs*: DAM and DEGSUN

*Catalogue number*: AAAK

*Computer*: CDC Cyber 76; *Installation*: Centro di calcolo interuniversitario dell'Italia Nordorientale, Casalecchio sul Reno BOLOGNA (Italy)

*Operating system*: scope 2.1.

*Programming language used*: FORTRAN IV

*High speed storage required*: 18 100 words

*No of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 361

*Keywords*: general purpose, representation, degeneracy, $U(n)$, unitary group, Lie algebra, weight, Gel'fand triangle

*Nature of the physical problem*
The importance of unitary symmetries in physics is well known. This program computes the multiplicity of a weight in a given irreducible representation of $U(n)$.

*Method of solution*
Given the rank $(n-1)$ of $U(n)$ the program DAM generates the program DEGSUN. This last program computes the multiplicity of the weight $m$ in a given irreducible representation of $U(n)$ by properties of the Gel'fand triangle.

*Typical running time*
Compile time was 14,610 s, total execution time for the test runs was 320, 733 s.

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Computer Physics Communications 14 (1978) 423–445
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# ATHENE 1: A ONE-DIMENSIONAL EQUILIBRIUM–DIFFUSION CODE

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and

J.W. LONG
*Oxford Polytechnic, Headington, Oxon OX3 0BP, UK*

Received 9 November 1977

## PROGRAM SUMMARY

*Title of program*: ATHENE 1

*Catalogue number*: ABUT

*Computer*: ICL 4/70; *Installation*: UKAEA Culham Laboratory. The program can be used on any computer equipped with the OLYMPUS system.

*Operating system*: ICL Multijob

*Programming languages used*: FORTRAN

*High speed store required*: 72 000 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 6698

*CPC Library subprograms used* *:

| *Catalogue number*: | *Title*: |
|---|---|
| ABUF | OLYMPUS (ICL 4/70) |
| ABUJ | OLYMPUS (IBM 370/165) |
| ABUK | OLYMPUS (CDC 6500) |

*Refs. in CPC*

| | |
|---|---|
| 7(1974) 245 | |
| 9(1975)51 | Alternative versions |
| 10(1975)167 | already published |

*Keywords*: plasma physics, thermonuclear fusion, pinch devices, reversed field pinches, one-dimensional, equilibrium, diffusion, implicit

*Nature of physical problem*
The purpose of ATHENE 1 is to calculate the evolution of a high-$\beta$ toroidal CTR plasma in the cylindrical approximation, taking into account diffusion and other entropy-generating processes in a plasma which evolves through a sequence of magnetohydrodynamic pressure equilibria. The ATHENE 1 model is intended mainly for calculations of plasma-pinch configurations.

*Method of solution*
The plasma and the magnetic field are described by five main

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* It is intended that the ATHENE 1 program should run under the OLYMPUS system, and that it should be used in conjunction with four general-purpose library packages FUNCON, COEFS1, CIRCE and OLYPOP. Until these four packages are published in the CPC Program Library, a Support File included at the end of the Program and Test Deck provides all the essential facilities that are required other than OLYMPUS itself.

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variables which are functions of the time $t$ and a single radial space variable $r$. The solution of the MHD equations in these five variables is split into two stages. In stage 1, which uses a fixed Eulerian mesh, diffusion and other processes change the entropy of the plasma-field configuration. Stage II is a Lagrangian calculation in which the calculation mesh is altered, so that the main variables undergo adiabatic changes until pressure equilibrium is reached. Only stage I of the calculation is described in detail here, stage II having been discussed in [1]. The four diffusion equations treated in stage I are solved by implicit integration schemes, and exact conservation of energy is ensured.

*Restrictions on the complexity of the problem*
Version 1 of ATHENE 1 provides a simple model for the behaviour of plasma-pinch configurations. A number of physical effects such as ionization and plasma impurities have been omitted, but additional physics can easily be included in the code, e.g. by use of the EXPERT facility [2,3]. In ATHENE 1 the initial radial profiles of the main variables can be altered as required. So too can the boundary conditions, and the exact conservation of energy provides a useful check against any error arising from modifications to the basic physics of the model. The accuracy of the solutions obtained for the main variables depends on the mesh size as well as on the choice of timestep.

*Typical running time*
Execution times depend on the amount of physics included in ATHENE 1 and also on the mesh size. The standard Test 1 described in the paper is carried out on a mesh with 20 cells and requires 150 s for 200 timesteps on the ICL 4/70 at Culham Laboratory.

*Unusual features of the program*
ATHENE 1 is written in OLYMPUS FORTRAN, i.e. Standard FORTRAN [4] except for the use of the NAMELIST facility. The structure of the code is based on the OLYMPUS system [2,3] in order to facilitate transfer to other types of computer. Subsets of the physics described in this paper can be excluded if appropriate logical switches are set.

It is intended that ATHENE 1 should be used in conjunction with four general-purpose library packages FUNCON (fundamental physical constants), COEFS 1 (plasma-diffusion coefficients), CIRCE (external circuits) and OLYPOP (OLYMPUS output package). Until these are available from the CPC Program Library, a Support File which is included at the end of the ATHENE 1 program deck provides all the essential facilities that are required other than OLYMPUS itself (see Appendix to this paper). Users who already have these packages may simply discard the corresponding module of the Support File.

*References*

[1] K.V. Roberts, J.P. Christiansen and J.W. Long, Comput. Phys. Commun. 10 (1975) 264.
[2] K.V. Roberts, Comput. Phys. Commun. 7 (1974) 237.
[3] J.P. Christiansen and K.V. Roberts, Comput. Phys. Commun. 7 (1974) 245.
[4] Standard Fortran Programming Manual (Computer Standard Series, National Computer Centre Ltd., Manchester, England, 1970).

Computer Physics Communications 15 (1978) 23–83
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# IMPACT, A PROGRAM FOR THE SOLUTION OF THE COUPLED INTEGRO–DIFFERENTIAL EQUATIONS OF ELECTRON–ATOM COLLISION THEORY

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Received 13 December 1977

## PROGRAM SUMMARY

*Title of program*: IMPACT

*Catalogue number*: ACYE

*Computer*: CDC 7600 (for test run); *Installation*: University of London Computer Centre. Also tested on CDC 6600, 6400 and IBM 360/65, 360/195, 370/165

*Operating system*: SCOPE 2.1.4 for test run.

*Programming language used*: FORTRAN IV

*High speed storage required*: 20 k words (decimal), with overlay

*No. of bits in a word*: 60

*Overlay structure*: overlaid for test run, overlay optional

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, 2 permanent disc files, 1 scratch disc file, punch optional

*Number of cards in combined program and test deck*: 6762

*CPC Library subprograms used*:

| *Catalogue number* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACYF | IMPPRO | This paper |

*Keywords*: atomic, electron–atom, electron–ion, scattering, structure

*Nature of the physical problem*
For a system containing $(M+1)$ electrons and a nucleus of charge $Z$, the wave function is taken to have the form [1]

$$\Psi = \sum_{i=1}^{\mathrm{NCHF}} \mathcal{A}\psi_i(M)\,\theta_i(1) + \sum_{j=1}^{\mathrm{NCHB}} \Phi_j(M+1)\,c_j\,, \tag{1}$$

where $\psi_i(M)$ is a wave function for the $M$ electron system; $\theta_i(1)$ is a one-electron wave function containing a radial function $F_i(r)$; $\mathcal{A}$ is an operator for anti-symmetrization and vector coupling; and $\Phi_j(M+1)$ is a wave function for the $(M+1)$ electron system. The condition is imposed that $\theta_i$ is orthogonal to all one-electron orbitals used in constructing $\psi_i$ and $\Phi_j$. It is required to obtain approximate solutions of the Schrödinger equation

$$\{H-E\}\,\Psi = 0\,. \tag{2}$$

Using a variational principle, one obtains a system of coupled integro–differential (ID) equations for the functions $F_i(r)$ and coefficients $c_j$ [1]. IMPACT is a computer program for the solution of these equations.

Put

$$E = \mathrm{ELOW} + \mathrm{EKLSQ}\,, \tag{3}$$

where ELOW is the energy for the ground state of the $M$ electron system and EKLSQ is input to the program. For EKLSQ $< 0$, IMPACT obtains approximate solutions of eq.

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[*] Permanent address: University College, London. M.J. Seaton is a Fellow-Adjoint of the Joint Institute for Laboratory Astrophysics.

[**] Now at Jesus College, Cambridge.

(2) for the bound state $\Psi_n$ of the $(M + 1)$ electron system with energy $E_n$ closest to ELOW + EKLSQ [3]. For EKLSQ > 0, IMPACT solves the corresponding electron–atom or electron–ion collision problem.

*Method of solution*
The radial functions $F_i(r)$ are tabulated at points

$$r = \mathrm{R}(1), \mathrm{R}(2), ..., \mathrm{R}(\mathrm{N}) \,, \qquad (4)$$

and matched to functions for $r > \mathrm{R(N)}$ obtained using a modified version of the program ASYM of Norcross [4]. Using numerical methods described in ref. [2], the ID equations are replaced by linear algebraic (LA) equations which are solved using standard techniques.

*Restrictions on the complexity of the problem*
The program IMPACT is provided in a form which must be pre-processed by a program IMPPRO [5], which inserts dimensions. Restrictions on the complexity of the problems which can be solved are determined entirely by available machine time and core store.

*Typical running time*
The test run is for the e + $C^{3+}$ problem with $\psi_i$ states $1s^2 2s$, $1s^2 2p$, and total angular momenta and parity $SL\pi$ = $^1P^0$. For three energies the time taken on the CDC 7600 at ULCC was 2.6 s.

Re-coding of the program ASYM has led to reduction by a factor between 2 and 4 in the time taken to obtain solutions in the asymptotic region.

*References*

[1] W. Eissner and M.J. Seaton, J. Phys. B: Atom. Molec. Phys. 5 (1972) 2187.
[2] M.J. Seaton, J. Phys. B: Atom. Molec. Phys. 7 (1974) 1817.
[3] M.J. Seaton and P.M.H. Wilson, J. Phys. B: Atom. Molec. Phys. 5 (1972) L1.
[4] D.W. Norcross, Comput. Phys. Commun. 1 (1969) 88.
[5] M.A. Crees, M.J. Seaton and P.M.H. Wilson, Comput. Phys. Commun. (1978), this paper.

## PROGRAM SUMMARY

*Title of program*: IMPPRO

*Catalogue number*: ACYF

*Computer*: CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: SCOPE 2.1.4

*Programming language*: FORTRAN IV

*High speed storage required*: 4 k words (decimal)

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, one scratch disc file, 2 permanent disc files, punch optional

*No. of cards in combined program and test deck*: 705

*Keywords*: pre-processor, editing, atomic, electron–atom, electron–ion, scattering, structure

*Nature of the physical problem*
IMPPRO is a preprocessor for the program IMPACT (this paper [1], catalogue number ACYE).

*Method of solution*
IMPPRO reads two cards. The first specifies files IT1, IT2 and IT3 and print level. File IT1 contains the unprocessed program IMPACT and file IT2 is used for scratch storage. The processed FORTRAN program IMPACT is written on file IT3. The second card specifies 8 basic dimension numbers for IMPACT and a parameter MACH for activation or de-activation of machine-dependent statements in IMPACT. IMPPRO computes subsidiary dimension numbers and, depending on the value of MACH, instructions for insertion or deletion of timing routines and optional insertion of CDC PROGRAM, OVERLAY and LEVEL2 statements. It calls a modified version of the UCL String Replacement Program [2].

*Restrictions on the complexity of the problem*
IMPPRO uses one character not in the standard FORTRAN character set. In CDC Standard Hollerith this is a 5,8-hole punch and is printed on CDC machines as "<".

*Typical running time*
2.7 s on the CDC 7600 at ULCC for processing of 6351 cards on file IT1.

*References*

[1] M.A. Crees, M.J. Seaton and P.M.H. Wilson, Comput. Phys. Commun. (1978), this paper.
[2] C. Day, Comput. Phys. Commun. 13 (1977) 101.

Computer Physics Communications 15 (1978) 85–96
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# SUBMMW: A THEORETICAL MODEL TO PREDICT CW SUB-MILLIMETER WAVE LASER PERFORMANCE

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Received 15 November 1977

## PROGRAM SUMMARY

*Title of program*: SUBMMW

*Catalogue number*: ACYC

*Computer*: IBM-360/91; *Installation*: NASA-Goddard Space Flight Center

*Operating system*: OS-360

*Programming language used*: FORTRAN

*High speed store required*: 53 K bytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line-printer

*No. of cards in a combined program and test deck*: 831

*Keywords*: laser, submillimeter wave, far infrared, gas laser, small signal gain, output power, absorption coefficient

*Nature of physical problems*
SUBMMW assumes that the energy levels of the lasing molecule are those of a symmetric top. The molecule is pumped by an intense laser source, for example, the $P(20)$ line of $CO_2$, from a rotational sub-level of one vibrational level to a higher vibrational level and then decays to a lower rotational level within the higher vibrational level emitting sub-millimeter wave radiation.

Given the parameters of the pump radiation, the constants associated with the lasing molecule, for example methyl fluoride, $CH_3F$, and the relaxation times, SUBMMW calculates small signal gain, saturated gain, output power and absorption coefficients. Consequently, the code can be used for *any* laser in which two lasing fields interact with a three level molecule.

*Method of solution*
The computer program solves the time-independent rate equation in a manner first developed by Tucker [1]. The theoretical model upon which SUBMMW is based is described in detail in Smith and Thomson [2]. The principal improvement over Tucker's model is the adaptation from the formalism of De Temple and Danielewicz [3] of terms representing absorption from the two travelling-wave components of the *pump* standing wave (which is usually measured in watts) rather than the FIR standing wave (which is usually present in the oscillator in milliwatts). The rate equations can be solved analytically leading to explicit formulae to be calculated for the gain and the absorption coefficient. These formulae involve an integral which must be evaluated with considerable care.

*Restrictions on the complexity of the problem*
This model of the C.W. SMMW laser programmed in SUBMMW involves the interaction of two laser fields with a three-level molecular system. Consequently, the model would have to be generalized to include
- (a) the effects of buffer gases;
- (b) to forecast the performance of pulsed systems;
- (c) the system of Hacker et al. [4] which involves five laser fields interacting with six molecular levels.

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* National Research Council Research Associate.

*Typical running time*
The two test cases took 0.02 mins of CPU and 0.03 mins of I/0 on the IBM-360/91.

*References*

[1] J.R. Tucker, Aerospace Technical Memorandum 74 (8170)-1, Aerospace Corporation, El Segundo, Calif. (1974).
[2] K. Smith and R.M. Thomson, Computer Modeling of Gas Lasers (Plenum Publ. Corp. 1978), sec. (9.3).
[3] T.A. De Temple and E.J. Danielewicz, J. Quant. Electron. 12 (1976) 40.
[4] M.P. Hacker, Z. Drozdowicz, D.R. Cohn, K. Isobe and R.J. Temkin, Phys. Lett. 57A (1976) 328.

Computer Physics Communications 15 (1978) 97–105
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# INTERACTIVE POSITRONFIT:
# A NEW VERSION OF A PROGRAM FOR ANALYSING POSITRON LIFETIME SPECTRA

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Received 16 January 1978

## PROGRAM SUMMARY

*Title of program*: INTERACTIVE POSITRONFIT

*Catalogue number*: AAHI

*Computer*: PDP 11; *Installation*: Queen's University, Canada

*Operating System*: RT-11 (Version 2-C)

*Programming language used*: FORTRAN

*High speed storage required*: 19 198 words

*No. of bits in a word*: 16

*Overlay structure*: main program plus three overlaid segments in one region

*No. of magnetic tapes required*: none

*Other peripherals used*: one teletype (or equivalent), one random-access storage device

*No. of cards in combined program and test deck*: 1367

*Reference to other published versions of this program*:

| *Cat. No.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAGX | POSITRONFIT EXTENDED | 7 (1974) 401 |
| AAGK | POSITRONFIT | 3 (1972) 240 |
| AAGZ | DBLCON | 13 (1978) 371 |

*Keywords*: positron, lifetime, time spectrum, least squares, fitting, interactive, convolution, resolution function, minimization, sum-of-exponentials, Marquardt, constraints, covariance matrix.

*Nature of the physical problem*
Positrons annihilate in condensed matter from different states (e.g. from defect traps in metals) so that a measured lifetime spectrum consists of a sum of exponential decay components smeared with the instrumental resolution function and superimposed on a constant background. Experimenters want to extract the lifetimes and intensities of the annihilation from different states.

*Method of solution*
Positron lifetime spectra are analysed by a weighted least-squares fitting to a model: a sum of exponentials, convoluted with a resolution function which is a sum of gaussians. Component lifetimes, relative intensities and time zero can be left free or constrained as in [1]. In addition, the gaussian widths of the resolution function and the total intensity can be free or constrained. Interactive recycling of the program, permitting a convenient change of data or fitting range, constraints, etc. is included.

*Restrictions on complexities of the problem*
Our memory size limit requires the following restrictions: four lifetime components, two gaussian functions in the resolution function, 150 channels in the spectrum, 120 channels analysed. These restrictions may be severe for some applications of this program (e.g. positronium studies), and can be lifted by increasing the length of various arrays.

*Unusual features of the program*
(1) The program is interactive and will run on a minicomputer (any minimum PDP-11 with 24 K of memory, supporting RT-11 and FORTRAN).

(2) An auxiliary program is included to generate a test file from the test deck.

*References*

[1] P. Kirkegaard and M. Eldrup, Comput. Phys. Commun. 7 (1974) 401.

[2] P. Kirkegaard and M. Eldrup, Comput. Phys. Commun. 3 3 (1972) 240.

Computer Physics Communications 15 (1978) 107–123
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# A PROGRAM FOR CALCULATING GAMMA–GAMMA DIRECTIONAL CORRELATION COEFFICIENTS AND ANGULAR DISTRIBUTION COEFFICIENTS FOR GAMMA RAYS OF MIXED MULTIPOLARITIES FROM PARTIALLY ALIGNED NUCLEI *

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and

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Received 6 January 1978

## PROGRAM SUMMARY

*Title of program*: THDST

*Catalogue number*: ABMZ

*Computer*: CDC 7600; *Installation*: Lawrence Livermore Laboratory, Livermore, California 94550

*Operating system*: FLOE

*Program language used*: FORTRAN IV

*High-speed storage required*: 41 353 words.

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, teletypewriter, disc, CRT data display

*No. of cards in combined program and test deck*: 1805

*Reference to other published version of this program*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ABPG | ANGCOR | 11 (1976) 75 |

*Keywords*: nuclear, spectroscopy, directional, correlation, mixing ratios, solid-angle corrections, orientation, directional distribution, chi-square, *F*-coefficient, Clebsch–Gordan coefficient, Legrendre polynomial, multipolarity, attenuation coefficients, angular-distribution coefficients, experiment, admixture

*Nature of the physical problem*
Conservation of angular momentum governs the multipolarity of electromagnetic transitions between nuclear excited states. In certain cases a mixture of two multipolarities may occur in a single transition. The amount of mixing, i.e. the mixing ratio, is determined by the structure of the nuclear levels involved. The most probable mixing ratio can be determined by accurately measuring the directional correlation between two transitions or the angular distribution of a gamma ray with respect to a beam of charged particles which partially aligns the nucleus.

The program ANGCOR [1], catalogue number ABPG, for analyzing gamma–gamma directional correlations has been modified to include analysis of the angular distribution data.

*Method of solution*
The program has two modes of operation. In mode I or data analysis mode, directional correlation or distribution coefficients $A_K$ are fit to the experimental data by the method of least-squares with second- and fourth-order Legendre polynomials having only even terms. The coefficients are then

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* Research supported in part by the US Department of energy under contract no. W-7405-Eng 48.

corrected for attenuation that is due to the experimental finite solid angles. For each spin sequence entered, a chi-square value is calculated for 49 possible values of each transition mixing ratio in the case of angular correlations. For angular distributions, a chi-square value is calculated for 49 possible values of the transition mixing ratio and for 49 values of $\sigma$, the half-width of a gaussian distribution that describes the partial alignment of the nucleus. At each point, $\chi^2$ is determined by comparing the properly normalized Legendre polynomial expansion with input data. The normalization is obtained from the $A_0$ coefficient that was determined in the first part of the calculation. Mode II, the data simulation mode, calculates a set of directional correlation coefficients either from spins and two mixing ratios or from a mixing ratio and a value of $\sigma$, corrects for solid angle, and calculates a set of angular correlation data normalized to $A_0 = 10\,000$. Assuming *Poisson* statistics, uncertainties are assigned to each calculated data point. These simulated data are then entered in mode I and result in a similar output. In effect, the second mode allows the user to test the program or to determine what results would look like for given spin sequences and mixing ratios or, in the case of an angular distribution, for a particular degree of partial alignment.

*Restrictions on the complexity of the program*
Input is restricted to ten angles or fewer. Correlations are limited to successive gamma-ray cascades.

*Typical running time*
Running time depends on the machine used and the number of angles entered. For input with seven angles and one-spin sequence, the running time on a CDC 7600 is approximately 1 s.

*References*

[1] E.S. Macias, W.D. Ruhter, D.C. Camp and R.G. Lanier, Comput. Phys. Commun. 11 (1976) 75.

Computer Physics Communications 15 (1978) 125–129
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# A PROGRAM FOR CALCULATING THE ANGULAR DISTRIBUTION OF NONRELATIVISTIC BREMSSTRAHLUNG INTENSITY

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*Universidad de Buenos Aires and Dirección General de Investigación y Desarrollo, Ministerio de Defensa,*
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Received 20 January 1978

## PROGRAM SUMMARY FORM

*Title of program*: BREMSSTRAHLUNG INTENSITY (NR)

*Catalogue number*: ACYJ

*Computer*: IBM 360/50; *Installation*: Servicio de Computación en Salud, Universidad de Buenos Aires

*Operating system*: DOS

*Programming languages used*: FORTRAN IV

*High speed store required*: 11328 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader; line printer

*No. of cards in combined program and test deck*: 300

*Keywords*: atomic, radiation, electron-ion, scattering, free-free transition, X-rays, nonrelativistic, bremsstrahlung, angular distribution, polarization components

*Nature of physical problem*
The program calculates the angular distribution of intensity for the bremsstrahlung emission with a given photon energy from ions at rest which are bombarded by electrons of known energy. The calculation is based on Sommerfeld's results [1], which are valid when shielding and relativistic effects are neglected.

*Method of solution*
The total bremsstrahlung intensity $I_t$ (integrated over all angles of observation $\phi$) is calculated by means of Weinstock's series expansion [2]. A fast convergent series [3] is used to evaluate one polarization component, e.g. $I_y$, whereby the other components ($I_x$, $I_z$) and the angular distribution $I(\phi)$ are straightforwardly obtained.

*Restrictions on the complexity of the problem*
The program is restricted to photon/electron energy ratios $R$ below $R_0 \simeq 0.97$, i.e. not close to the high energy limit. A rather large number of terms in the series expansions is required when the ratio $R$ is larger than 0.95. For all other values of $R$ the only restrictions arise from the error in the available values of physical constants [4], which amounts to less than 10 ppm. Electron energies out of the physical range of interest for bremsstrahlung emission ($U/Z^2 < 0.0001$ keV, with $U$ = incident electron energy, $Z$ = target ion atomic number) may result in an underflow condition.

*Typical running time*
Running times range between ~1 s for moderate energy values and ratios ($E = U/Z^2 = 0.001$ to 100 keV; $R = 0.01$ to 0.85) and ~20 s for high energy ratios ($R \lesssim 0.95$), with EPS = $10^{-20}$.

*References*
[1] A. Sommerfeld, Ann. Phys. 11 (1931) 257.
[2] R. Weinstock, Phys. Rev. 61 (1942) 584.
[3] A. Bañuelos and F. Rodríguez-Trelles, J. Phys. B, to be published.
[4] Particle Data Group, Rev. Mod. Phys. 48 (1976) S 35.

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Computer Physics Communications 15 (1978) 131–145
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# GENERATION OF THE CLEBSCH–GORDAN COEFFICIENTS FOR $S_n$ *

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and

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Received 6 August 1976
Received in revised form 24 January 1978

## PROGRAM SUMMARY

*Title of program*: SYMCGM

*Catalogue number*: ACXV

*Computer*: IBM 370/168; *Installation*: City University of New York University Computing Center

*Operating system*: OS/MVT/ASP

*Programming language used*: FORTRAN IV

*High speed storage required*: 252 kbytes (for (6,6,6) triplet of $S_6$)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required (if used)*: 2

*Other peripherals used*: card reader, line printer, card punch or tapes

*No. of cards in combined program and test deck*: 1876

*CPC library subprograms used (for data)*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACXW | SYMFUNC | this issue |

*Keywords*: general purpose, symmetric group, Clebsch–Gordan coefficients, tensor product, decomposition, irreducible representation

*Nature of physical problem*
To find the decomposition of the tensor product of two irreducible representations of the symmetric group $S_n$ (for any $n$) into a direct sum of irreducible representations, and to compute the matrices for the similarity transformations.

*Method of solution*
An iterative formula [1] has been derived which gives the tensor coupling coefficients for $S_n$ in terms of the Clebsch–Gordan coefficients for $S_{n-1}$ and the matrix elements for the transposition $(n-1\ n)$. The computation is then essentially by direct substitution. Symmetry relations are used to reduce the number of coefficients which need to be calculated. The Clebsch–Gordan coefficients are then found from the tensor coupling coefficients by methods previously developed [1].

*Restrictions of the size of the problem*
These are determined by the amount of storage space and

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* Supported by City University of New York Educational Computer Center.

running time allotted. For large $n$ the imprecision of the coefficients can be greater than their magnitude. The values of $n$ for which the program works can be increased by using greater precision. If $n$ is greater than 12 the integer format of the function FAC will have to be changed. With the values presently specified in the dimension statements the program will work for all $n$ through 5 and in addition for all triplets for $n = 6$. However, the larger triplets will have to be done individually.

*Unusual features of the program*
Since this is an iterative procedure the coefficients for $S_{n-1}$ must be stored for use in calculating those for $S_n$. This requires a large amount of storage. The program is designed to store only the non-zero coefficients. Symmetry properties allow the calculation and storage of only a subset of these. Thus, a large part of the program consists of search routines for finding coefficients.

*Reference*

[1] S. Schindler and R. Mirman, J. Math. Phys. 18 (1977) 1678.

## PROGRAM SUMMARY

*Title of program*: SYMOR

*Catalogue number*: ACYH

*Computer*: IBM 370/168; *Installation*: City University of New York University Computing Center

*Operating system*: OS/MVT/ASP

*Programming language used*: FORTRAN IV

*High speed storage required*: 102 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of tapes required (if used)*: 1

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 176

*CPC library subprograms used (for data)*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACXV | SYMCGM | this paper |

*Keywords*: general purpose, symmetric group, orthonormality, precision

*Nature of physical problem*
The Clebsch–Gordan coefficients of the symmetric group obey certain orthonormality conditions [1]. This program checks to see that the coefficients computed do actually obey these conditions. The deviation from exact orthonormality also provides a useful estimate of the accuracy of the calculation and the precision of the coefficients. Note that the calculational procedure of SYMCGM does not force orthonormality, except to some extent, for multiplicity greater than one, for $r_0$ (=1).

*Method of solution*
The program is closely related to SYMCGM described in this paper and the notation and routines generally follow that program. Its input is the output of SYMCGM, and a single data card, similar to that for SYMCGM.

For each triplet a vector is specified by a tableau index and a multiplicity index. All pairs of vectors in the triplet, are considered and the dot product for each pair calculated.

The output is headed by the value of $n$ and the triplet indices. Then a line appears for each pair of vectors giving the trableau index for each vector, the multiplicity index for each, and then the value of the dot product. This dot product should be one if all the indices are the same and zero otherwise.

*Restrictions on the complexity of the problem*
Any coefficient computed by SYMCGM can be checked.

*References*

[1] S. Schindler and R. Mirman, J. Math. Phys. 18 (1977) 1678, eq. V-6.

## PROGRAM SUMMARY

*Title of program*: SYMCC

*Catalogue number*: ACYI

*Computer*: IBM 370/168; *Installation*: City University of New York University Computing Center

*Operating system*: OS/MVT/ASP

C-492

*Programming language used*: FORTRAN IV

*High speed storage required*: 246 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of tapes required (if used)*: 1

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 267

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACXV | SYMCGM | This paper |
| ACXW | SYMFUNC | This issue |

*Keywords*: general purpose, symmetric group, homogeneous equations, precision

*Nature of physical problem*

The Clebsch–Gordan coefficients of $S_n$ must satisfy certain homogeneous equations [1]. The program SYMCGM described in this paper computes thse coefficients and SYMCC checks that the computed coefficients actually satisfy the equations. In addition, SYMCC provides some indication of the accuracy of the calculation and the precision of the coefficients.

*Method of solution*

The program SYMCC is closely related to SYMCGM, in general, following its notation and routines. Its input is the output of that program, as well as output from SYMFUNC [2], and a single data card. The information and setting of indices for $n$ and a triplet is the same as for SYMCGM. The data card also contains two other numbers (NSK) and (LST).

The homogeneous equations can be checked for all the neighboring transpositions or only the last one as specified by the variable (NSK)

The difference between the values of the two sides of each equation (which should be zero) is computed. For each neighboring transposition the sum of the absolute values of the differences, and the largest absolute value of all the differences are found.

The output is headed by the label of the neighboring transposition and the triplet indices. Then, for each set of indices there is a line listing the indices, the values of the right- and left-hand sides and the difference. Instead of every line being printed, only every (LCT) lines can be printed.

After all this information is the sum, and the largest, of the absolute values of the differences.

*Restrictions on the complexity of the problem*

Any coefficient computed by SYMCGM can be checked.

*References*

[1] S. Schindler and R. Mirman, J. Math. Phys. 18 (1977) 1678, eq. VIII-7, and sec. IX.

[2] S. Schindler and R. Mirman, Comput. Phys. Commun., 15 (1978) 147; a slightly modified version of SYMFUNC produces the required data. The procedures for modifying it are stated in that program.

Computer Physics Communications 15 (1978) 147–152
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# FUNCTIONS ON TABLEAUX AND FRAMES OF THE SYMMETRIC GROUP *

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and

R. MIRMAN
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Received 6 August 1976
Received in revised form 24 January 1978

## PROGRAM SUMMARY

*Title of program*: SYMFUNC

*Catalogue number*: ACXW

*Computer*: IBM 370/168; *Installation*: City University of New York University Computing Center

*Operating system*: OS/MVT/ASP

*Programming language used*: FORTRAN IV

*High speed storage required*: 138 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of tapes required (if used)*: 1

*Other peripherals used*: card reader, line printer, card punch or tapes

*No. of cards in combined program and test deck*: 805

*CPC library subprograms used*: none

*Keywords*: general purpose, symmetric group, irreducible representation, frame, tableau

*Nature of the physical problem*:
To compute data needed for SYMCGM [1], specifically, the row and column lengths and the dimensions of the frames, the orthogonal matrices and sign functions

*Method of solution*
The specific algorithms have been discussed in refs. [2] and [3].

*Restrictions on the complexity of the problem*
Any date needed by SYMCGM [1] can be computed

*Typical running time*
Through $S_6$ : 0.425 min.

*References*

[1] S. Schindler and R. Mirman, Comput. Phys. Commun., preceding paper.
[2] S. Schindler and R. Mirman, J. Math. Phys. 18 (1977) 1678.
[3] S. Schindler and R. Mirman, J. Math. Phys. 18 (1977) 1697.

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* Supported by City University of New York Educational Computer Center.

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Computer Physics Communications 15 (1978) 165–192
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# A-THREE: A GENERAL OPTICAL MODEL CODE ESPECIALLY SUITED TO HEAVY-ION CALCULATIONS [*]

E.H. AUERBACH
*Brookhaven National Laboratory, Upton, New York 11973, USA*

Received 15 October 1977

## PROGRAM SUMMARY

*Title of program*: A-THREE

*Catalogue number*: ABII

*Computer*: CDC-7600; *Installation*: Central Scientific Computing Facility, Brookhaven National Laboratory

*Operating system*: CDC Scope 2.1

*Programming language used*: FORTRAN-extended

*High speed storage required*: 21 500 words (small core only)

*No. of bits in a word*: 60

*Overlay structure*: six overlays ("root" and one level)

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, punch (optional), magnetic disc (optional)

*No. of cards in combined program and test deck*: 3571

*Keywords*: nuclear, optical model, complex potential, elastic, scattering, heavy-ions, Schrödinger equation, phase shifts, nuclear bound states

*Nature of physical problem*
The non-relativistic radial Schrödinger equation with complex potential is solved partial wave by partial wave to obtain phase shifts, from which total (reaction) cross sections, elastic scattering angular distributions and polarization angular distributions are obtained. Optionally, radial wave functions may be retained. The complex optical potential may take a large number of forms and may, also, have the parts of the potential read in (from other calculations) or calculated by user supplied subroutines. Within the same structure, bound states for a real potential may be calculated.

Provision is made to search (a) for an eigenvalue or potential which produces a given eigenvalue in the bound state case, and (b) to fit given data or sets of data, with or without angular resolution, in the scattering case. The parameter space may also be "scanned", without search.

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[*] Work supported by United States Department of Energy under Contract no. EY-76-C-02-0016.

*Method of solution*
The radial differential equation is integrated by the Noumerov method (with mesh refinement, if necessary); the principal search method is a variable metric minimization after Fletcher-Powell and Davidon [1].

*Restrictions on the complexity of the problem*
Partial waves are limited to $l = 800$ for no spin and $l = 400$ with spin; the total number of partial waves actually computed is limited to 400, absorption for the lower uncomputed partial waves being set to 1.0. Potential specification must be made in an equally spaced grid of not over 500 intervals.

*Special features*
All arrays requiring more significant figures than 32-bit machines allow are noted; similarly for alphanumeric words of more than four characters.

*References*

[1] R. Fletcher and M.J.D. Powell, Comput. J. 6 (1969) 163.

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# A FINITE RANGE COUPLED CHANNEL BORN APPROXIMATION CODE

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and

R.D. KOSHEL **
*Physics Department, Ohio University, Athens, Ohio 45701, USA*

Received 4 December 1977

## PROGRAM SUMMARY

*Title of program*: FRCCBAOUKID

*Catalogue number*: ABPI

*Computer*: CDC 6600/Cyber 74; *Installation*: Florida State University

*Operating system*: CDC-Kronos

*Programming language used*: FORTRAN IV

*High speed storage required*: 75 kwords (Octal)

*No. of bits in a word*: 60

*Overlay structure*: yes

*No. of magnetic tapes required*: none

*Other peripherals used*: disk storage, card reader, line printer

*No. of cards in combined program and test deck*: 3217

*Keywords*: nuclear, coupled channels, Born approximation, finite range, direct reactions, heavy ions, plane wave expansion

*Nature of the physical problem*
The computer code OUKID calculates differential cross sections for direct transfer nuclear reactions in which multistep processes, arising from strongly coupled inelastic states in both the target and residual nuclei, are possible. The code is designed for heavy ion reactions where full finite range and recoil effects are important.

*Method of solution*
Distorted wave functions for the elastic and inelastic scattering are calculated by solving sets of coupled differential equations using a Matrix Numerov integration procedure [1]. These wave functions are then expanded into bases of spherical Bessel functions by the plane-wave expansion method [2]. This approach allows the six-dimensional integrals for the transition amplitude to be reduced to products of two one-dimensional integrals. Thus, the inelastic scattering is treated in a coupled channel formalism while the transfer process is treated in a finite range born approximation formalism.

*Restrictions on the complexity of the problem*
(1) No more than three states can be coupled in each the target and the residual nucleus.
(2) The projectile and the target nuclei cannot be simultaneously excited.
(3) The wave number for the relative kinetic energy should be less than 5 $\mathrm{fm}^{-1}$.
(4) No more than 90 partial waves are allowed.
(5) Coulomb excitation is not included.
(6) The transferred particle is assumed to be a cluster with no internal structure.

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* Work supported in part by the National Science Foundation, Grants nos. NSF-GU-2612, NSF-PHY-74-02673, and NSF-GJ-367.
** Work supported in part by the National Science Foundation, Grant no. NSF-PHY-77-03662.

*References*

[1] M.A. Melkanoff, T. Sawada and J. Raynal, Methods in Computational Physics, vol. 6 (Academic Press, 1966) p. 1.

[2] P. Griffin, P. Nagel and R.D. Koshel, J. Math. Phys. 15 (1974) 1913.

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Computer Physics Communications 15 (1978) 227–235
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# NEW FORTRAN PROGRAMS FOR ANGULAR MOMENTUM COEFFICIENTS

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and

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Received 16 January 1976; in revised form 21 November 1977

## PROGRAM SUMMARY

*Title of program*: ANGMOM

*Catalogue number*: ACYK

*Computer*: IBM 370/168; *Installation*: University of Bonn Computation Centre

*Operating system*: OS-VS2

*Programming language used*: FORTRAN IV(G)

*High speed store required*: 14544 words

*No. of bits in a word*: 32 (4 bytes)

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader and line printer

*No. of cards in combined program and test deck*: 904

*Keywords*: general purpose, nuclear, atomic, molecular, angular momentum, nuclear structure, nuclear reactions, matrix element, Clebsch–Gordan coefficient, Racah coefficient, high spin states, coupling and recoupling coefficients, shell model, generalized hypergeometric functions, rotation group

*Nature of the physical problem*
The program calculates the Clebsch–Gordan and Racah coefficients, using conventional formulae [1], the improved codes due to Wills [2] and Bretz [3] and in terms of generalized hypergeometric functions of unit argument defined by us [4,5]. The Clebsch–Gordan coefficient arises in the coupling of two angular momenta and the Racah coefficient arises in the recoupling of three angular momenta. These coefficients are of fundamental importance in nuclear, atomic and molecular physics calculations.

*Method of solution*
In refs. 4 and 5 we have shown that a set of six ${}_3F_2(1)$s and two equivalent sets of ${}_4F_3(1)$s are necessary and sufficient to account, respectively, for the known symmetries of the Clebsch–Gordan and Racah coefficients. Wills [2] has shown that the conventional approach detailed by Tamura [6], when used for large values of angular momenta, will lead, in single-precision, to inaccurate results due to the computer round-off error and he proposed an improved method which is more accurate and faster. The hypergeometric functions have this improvement naturally built-in and their use for the Clebsch–Gordan and Racah coefficients yields new FORTRAN programs which are shown here to yield the same accuracy as that attained by Wills [2] and Bretz [3] and are even faster.

*Typical running time*
The execution time required to calculate a Clebsch–Gordan or a Racah coefficient depends mainly upon the values of

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[*] On leave of absence from: MATSCIENCE, The Institute of Mathematical Sciences, Madras-600 020, India.

its arguments. For small values of angular momenta, the conventional method of Tamura [6], the method of Wills [2] and Bretz [3] and our methods all yield the same results. But, for large values of angular momenta, in single-precision, while Tamura's method [6] breaks down due to large round-off errors, the Wills [2] –Bretz [3] method is not only more accurate but is approximately twice as fast as Tamura's method with negligibly small round-off errors. Our programs based on the use of generalized hypergeometric functions and their properties, are as accurate as those of Wills and Bretz and are even faster than their programmes by about 5–15%.

*References*

[1] G. Racah, Phys. Rev. 62 (1942) 438.
[2] J.G. Wills, Comput. Phys. Commun. 2 (1971) 381.
[3] V. Bretz, Acta Phys. Acad. Sci. Hungaricas 40 (1976) 255.
[4] K. Srinivasa Rao, Proc. 6th Int. Coll. on Gp. Theor. Methods in Phys., Tübingen (1977) and to be published.
[5] K. Srinivasa Rao, T.S. Santhanam and K. Venkatesh, Jour. Math. Phys. 16 (1975) 1528 and K. Srinivasa Rao and K. Venkatesh, Proc. of 5th Int. Coll. on Gp. Theor. Methods in Phys., Montreal (1976).
[6] T. Tamura, Comput. Phys. Commun. 1 (1970) 337.

Computer Physics Communications 15 (1978) 237–245
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# A FORTRAN PROGRAM FOR ROUTINE ANALYSIS OF MAGNETIC SUSCEPTIBILITY DATA

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*The University of Akron, Akron, Ohio 44325, USA*

Received 2 March 1978

## PROGRAM SUMMARY

*Title of program*: SUSCEPT2

*Catalogue number*: ABNA

*Computer*: IBM 370/158; *Installation*: The University of Akron, Akron, Ohio 44325, USA

*Operating system*: OS/VS2; OS/MVS

*Programming language used*: FORTRAN IV (G1)

*High-speed store required*: 10000 words (40 kbt) exclusive of loader

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: Card reader, line printer

*Number of cards in combined program and test deck*: 747

*Keywords*: Solid state, magnetism, magnetic susceptibility, Faraday method, Curie–Weiss law, ferromagnetic correction, temperature-independent susceptibility, chi-square, fit.

*Nature of physical problem*
Faraday susceptibility data in the form of balance readings are converted to susceptibilities, and optionally interpreted in terms of a Curie–Weiss temperature dependence.

*Method of solution*
Susceptibilities $\chi$ are calculated from the data *via* their definition; ferromagnetic corrections are made using a two-point extrapolation of $\chi(H)$ vs. $1/H$ to infinite field; Curie–Weiss interpretation is done on the results of a least-squares fit of $\chi^{-1}$ vs. $T$, where a temperature-independent $\chi_0$ can also be fitted.

*Restrictions on program complexity*
The present limit of 100 data points is easily extended.

*Typical running time*
On the IBM 370/158, the program compiles (G1 compiler) in about 8 CPU s. A typical case with full interpertation takes less than 3 CPU s.

*Unusual features of the program*
(1) For each temperature, $\chi$ values at one or two magnetic fields are found, with uncertainties, corrected for the weight and magnetism of sample supports. If $\chi$ is given at two fields, values are averaged or a ferromagnetic correction applied, as appropriate. A constant $\chi_0$ value, if supplied, is subtracted from all points.
(2) A calibration mode calculates apparatus constants given a sample of known susceptibility. Constants stay in effect until the next calibration; defaults may be provided.
(3) A fit of the data to the equation $\chi - \chi_0 = C/(T - T_c)$ is optional, yielding $C$, $T_c$, and optionally $\chi_0$, above a cut-off temperature $T_{cut}$ which may be zero, specified, or derived from the fit.
(4) Line printer plots of $\chi$ vs. $T$ (and $\chi^{-1}$ vs. $T$ with the Curie–Weiss fit) are provided.

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# FINE STRUCTURE CROSS SECTIONS FROM REACTANCE MATRICES – A MORE VERSATILE DEVELOPMENT OF THE PROGRAM JAJOM

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Received 18 January 1978; in revised form 4 April 1978

## PROGRAM SUMMARY

*Title of program*: JAJOMPRE

*Catalogue number*: ACYG

*Computer*: IBM 360/65, IBM 360/195, CDC 6400; *Installation*: University College London, SRC/Rutherford Laboratory, UK, JILA, University of Colorado

*Operating system*: OS 360, scope 3.4

*Programming language used*: FORTRAN IV

*High speed store required*: 90760 bytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 2835

*Reference to other published version of this program*: Cat. No.: AAGJ; Title: JAJOM; Comput. Phys. Comm. 3 (1972) 256

*Keywords*: Atomic, electron–atom, scattering, reactance matrices, pair coupling, collision strengths

*Nature of physical problem*
Results from calculations with *LS*-coupled wave functions (reactance matrices and term coupling coefficients) are used to compute collision strengths for transitions between fine structure levels.

*Method of solution*
The input is carefully checked. The algebraic transformation uses Racah algebra, the coefficients are computed as required. An optional further transformation to allow for intermediate coupling in the target requires term coupling coefficients to be supplied by the user. The collision strengths are computed using either of two formulae, corresponding to weak or strong coupling respectively.

*Unusual features of the program*
This version of JAJOM is very flexible. Using the preprocessor included with this deck machine dependent features, array lengths, and mode of operation are all inserted according to the user's requirements.

*Restrictions on the complexity of the problem*
It is not recommended to use the program for angular momenta greater than about 20. But adaptations are possible by replacing the Racah algebra subroutines. We discuss addition of contributions from high angular momenta using approximate methods. For problems with a large number of target levels the execution time can become large; a comment card in MAIN points to a place where a RESTART procedure can conveniently be inserted.

*Typical running time*
We give two sets of sample runs, which took 12 and 27 s respectively on the IBM 360/65.

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# II. REDUCED SU(3) MATRIX ELEMENTS *

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*Dept. of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA*

Received 8 February 1978

## PROGRAM SUMMARY

*Title of program*: REDUCED SU(3) MATRIX ELEMENTS

*Catalogue number*: ABKH

*Computer*: AMDAHL 470V/6, IBM 360/370; *Installation*: Univ. of Michigan, Ann Arbor, Mich.

*Operating system*: MTS

*Program language used*: FORTRAN

*High speed storage required*: 212 kwords

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer (card punch)

*No. of cards of combined program and test deck*: 907

*CPC library programs used*:

*Catalogue number*: ABKG

*Title*: REDUCED SU(3) CFPS

*Ref. in CPC*: 14 (1978) 109

*Catalogue number*: AAC*

*Title*: DATA FOR ABKG

*Ref. in CPC*: 14 (1978) 109

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* Work supported by the U.S. National Science Foundation.

** Present address: Goddard Space Flight Center, Seabrook, MD, USA.

*Keywords*: Nuclear physics, SU(3), SU(4), shell model, matrix elements, nuclear structure, pseudo-SU(3), one-body operators, two-body operators, theoretical methods

*Nature of physical problem*

Reduced SU(3) matrix elements (RME) are calculated for a general one or two body tensor operator, between arbitrary shell model states in an SU(3) × SU(4) or SU(3) × SU(2) scheme. Matrix elements in the angular momentum scheme can then be obtained by multiplying these RME with the appropriate SU(3) ⊃ R(3) coupling coefficients available through the code of ref. [2].

*Method of solution*

One and two body tensor operators are explicitly constructed in terms of fermion creation operators. Since the ⟨BRA| and |KET⟩ states obtained by using the appropriate routines of the code of ref. [1] are also written in terms of fermion creation operators, the overlap can be calculated directly. This method is typically 2–3 orders or magnitude faster than the usual CFP expansion.

*Restrictions on the complexity of the problem*

The ⟨BRA| and |KET⟩ states are restricted to those that can be calculated with the code of ref. [1]. No other restrictions exist.

*Unusual features of the program*

The same array naming convention adopted in the code of ref. [1] is kept. This allows a saving of up to 35% of high speed storage in IBM 360/370 or similar operating systems.

*References*

[1] D. Braunschweig, Comput. Phys. Commun. 14 (1978) 109.
[2] Y. Akiyama and J.P. Draayer, Comput. Phys. Commun. 5 (1973) 405.

Computer Physics Communications 15 (1978) 275–282
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# AN ADAPTATION OF ACRZ TO CALCULATE ELECTRIC QUADRUPOLE OSCILLATOR STRENGTHS

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Received 17 February 1978; in revised form 14 April 1978

## ADAPTATION SUMMARY

*Title of adaptation*: QUADRUPOLE TRANSITIONS

*Adaptation number*: 0001

*Catal. number*: ACRZ *Title*: GF VALUES *Ref. in CPC*: 9 (1975) 381

*Authors of original program*: C. Froese Fischer and K.M.S. Saxena

*Computer*: CDC 6600; *Installation*: Université Libre de Bruxelles, Brussels, Belgium

*Operating system*: NOS 1.0

*Programming language used in adapted program*: FORTRAN IV

*High speed core required*: 45600 (octal) words

*Number of bits in a word*: 60

*No. of cards required to effect adaptation (including directive cards)*: 430

*CPC library subprograms used (to supply data)*:
*Catalogue number*: ACRF
*Title*: MCHF72
*Refs. in CPC*: 4 (1972) 107; 7 (1974) 236
*Catalogue number*: AAKP
*Title*: REDUCED TENSOR MATRIX ELEMENTS 2
*Ref. in CPC*: 9 (1975) 370

*Additional keywords*: electric multipole transitions, off-diagonal hypervirial theorem

*Nature of physical problem*
The adaptation allows the calculation of quadrupole electric oscillator strengths using results from MCHF72 [1]. The program REDUCED TENSOR MATRIX ELEMENTS 2 of Froese Fischer and Saxena [2] provides some additional input data for the calculation (the addition of 2 cards to this program allows the order $\chi$ of the tensor to be punched out). The first two forms of the hypervirial theorem [3] are computed.

*Method of solution*
The radial functions are given in tabular form and the integrals are evaluated numerically. Simpson's rule is used for the first form of the hypervirial theorem as in the dipole case $\chi = 1$ and we have applied the special formula already derived for the velocity form of the dipole operator to the quadrupole operator.

*Restriction on the complexity of the problem*
The restrictions concerning the dimensions of the arrays and the inclusion of maximum three overlap integrals (appearing due to the non-orthogonality between the orbitals of initial and final states) are the same as those in the original program [2].

*Typical running time*
The CPU time required for the calculations of the test run is 1.88 s on the CDC 6600 system.

*References*

[1] C. Froese Fischer, Comput. Phys. Commun. 4 (1972) 107; 7 (1974) 236.
[2] C. Froese Fischer and K.M.S. Saxena, Comput. Phys. Commun. 9 (1975) 370.
[3] J.C.Y. Chen, J. Chem. Phys. 40 (1964) 615.

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# CARLA: A CODE TO CALCULATE THE POPULATION OF HIGH SPIN STATES THROUGH COMPOUND NUCLEUS REACTIONS

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*Istituto di Fisica and INFN, Padova, Italy*

Received 8 August 1977; in revised form 10 April 1978

## PROGRAM SUMMARY

*Title of program*: CARLA

*Catalogue number*: ABGQ

*Computer*: CDC 7600; *Installation*: Centro di Calcolo Interuniversitario dell'Italia Nord-Orientale, Bologna

*Operating system*: SCOPE 2.1.3.

*Programming language used*: FORTRAN IV

*High speed storage required*: 25320 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, disc

*No. of cards in combined program and test deck*: 1085

*Keywords*: Nuclear physics, reaction, compound nucleus, Hauser–Feshbach, level density, yrast level, high spin state

*Nature of physical problem*
Calculation of the direct population of high spin state in the frame of statistical model.

*Method of solution*
The absolute cross section was calculated evaluating the integrals with the first order Gauss-Legendre method.

*Restrictions on program complexity*
Emission of a maximum of 3 particles of the type n,p,$\alpha$ (the formula used is repetitive, but for more than 3 particles the calculation increases greatly). The population of 10 levels by seven different beam energies may be obtained at one time.

*Typical running time*
This time is strongly dependent on the required calculations.

*Unusual feature of the program*
The program calculates the direct population of level.

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# MUONIC ATOM CASCADE PROGRAM *

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Received 19 December 1977; in revised form 27 February 1978

## PROGRAM SUMMARY

*Title of program*: MUONIC ATOM CASCADE

*Catalogue number*: AAMA

| *Computer*: | *Installation*: |
|---|---|
| CDC6600, 7600 | Berkeley, CA |
| IBM370/158 (MVS) | CALTECH, Pasadena, Ca * |
| PDP-10 (KA-603 Monitor) | CALTECH, Pasadena, Ca * |

*Remarks*:
* with minor modifications

*Operating system*: BKY24B-V2 system (FTN4 compiler, OPT = 2)

*Programming language*: FORTRAN IV

*High speed store required*: 30 kwords

*No. of bits in a word*: 32 (IBM), 36 (PDP), 60 (CDC)

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line-printer (120 position wide), card punch (optional)

*No. of cards in combined program and test deck*: 2760

*Keywords*: Atomic physics, negative muon, cascade, Auger, radiative, polarization, X-rays, multipole, angular momentum, monopole, dipole, quadrupole, octupole, shells, depolarization, penetration.

*Nature of physical problem*
The radiative and Auger transition rates of a negative muon in an atomic cascade, as well as the muon depolarization are calculated; the intensities of X-rays are calculated, sorted and printed. User selected transitions and their intensities are optionally punched.

*Method of solution*
Using the multipole radiative and Auger transition rates and an initial distribution of angular momentum of the negative muon, the population of the final states and the intensities of the resulting muonic X-rays are calculated in a systematic way and a catalogue of X-ray intensities is printed. This program is an upgraded version of an earlier work [1], with the following improvements: 1) Complete monopole, dipole, quadrupole, and octupole treatment, 2) K, L and M shells are included for all multipolarities, 3) Penetration is included in all cases, 4) The muon depolarization due to the spin-orbit coupling is calculated, 5) The input and output options are flexible. The underlying principles are discussed in the long writeup and in the thesis of one of the authors [2].

*Typical running time*
58.0 s on CDC7600 (including 8.1 s to compile and load) for one full cascade with mainly default options (multipoles up to $\lambda = 3$, penetration included with cutoff at $y = 1$) starting from principal quantum number 18. The running time will depend very strongly on the starting principal quantum number (proportional to a power between 4 and 5 thereof), on the length of the X-ray intensity catalogue, and on the other options selected (mainly on the treatment of penetration).

*References*
[1] J. Hufner, Z. Phys. 195 (1966) 365.
[2] V.R. Akylas, Ph.D. Thesis, CALTECH (1978) unpublished

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* Work supported by Department of Energy Contract EY-76-C-03-0063.

Computer Physics Communications 15 (1978) 351–373
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# NULLIJN, A PROGRAM TO CALCULATE ZERO CURVES OF A FUNCTION OF TWO VARIABLES OF WHICH ONE MAY BE COMPLEX

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Received 25 January 1978; in revised form 14 April 1978

## PROGRAM SUMMARY

*Title of program*: NULLIJN

*Catalogue number*: ACYL

*Computer*: CDC Cyber 73/173; *Installation*: Academic Calculation Centre, Amsterdam (SARA)

*Operating system*: NOS/BE 1.1

*Program language used*: FORTRAN IV (Compass intermixed)

*High speed storage required*: 51 kwords

*No. of bits in a word*: 60

*Overlay structure*: overlaid, can easily be removed

*No. of magnetic tapes required*: none

*Other peripherals used*: lineprinter, card reader or interactive terminal, plotter, disk

*No. of cards in combined program and test deck*: 4092

*Keywords*: general purpose, implicity defined function, zero curve, graphics, plasma dispersion, potential problems

*Nature of physical problem*
When an algorithm for a function $f$ of two variables, for instance a dispersion function $f(\omega, k)$ or a potential $V(r, z)$, is known, the program calculates and plots the zero curves, thus giving a graphical representation of an implicitly defined function. One of the variables may be complex.

*Method of solution*
A quadratic extrapolation, followed by a regula falsi algorithm to find a zero is used to calculate a succession of zero-points along a curve. The starting point of a curve is found by detecting a change of sign of the function on the edge of the area $G$ that is examined.

*Restrictions*
Curves that lie entirely inside $G$ are not found. Starting points of curves where the imaginary part of the complex variable is large might be missed.

*Typical running time*
The running time depends on the kind of function that is investigated. The algorithm for the evaluation of the function is usually executed 2 000–30 000 times.

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Computer Physics Communications 15 (1978) 375–386
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# SIMULATION OF ULTRASONIC DEGRADATION OF MACROMOLECULES IN SOLUTION

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Received 6 January 1978; in revised form 25 April 1978

## PROGRAM SUMMARY

*Title of program*: USSI

*Catalogue number*: ACYN

*Computer*: IBM 370/158; *Installation*: University of Liège

*Program language used*: FORTRAN IV

*High speed storage required*: 96 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 792

*Keywords*: ultrasonation, macromolecular solution, degradation rate, molecular weight distribution, simulation

*Nature of the physical problem*
Two main aspects are to be considered in ultrasonic degradation of polymers in solution:

- what is the rate of chain breakage?
- where are the points of breakage located along the polyme chain?

The study of the degradation process is based on the dete mination of the molecular weight distribution (polydispersity PDIS) and of an average molecular weights (number AMWN or weight AMWW **) as a function of the irradiation time. We have compared these experimental data with simulated values obtained by computer, for testing different hypothese concerning the rate expression and the breakage model.

Some simulation programs have been reported [1–3], but, so far as we know, have never been published. Our program is designed to be very general and the four breakage models programmed should cover most of the possible cases.

*Method of solution*
The method used to simulate ultrasonic action on polymers is quiet simple: we start from the initial molecular weight distribution and we follow during the time, how the number of molecules of each length is modified by breakage and redistribution of broken segments.

The program USSI is convenient for testing a large numbe of rate expression and breakage models.

*Typical running time*: 58 s.

*Unusual features*
ENTRY statements are used to optimise computation; however we have enclosed comments ("C****** instruction") to help users to suppress the ENTRY statements if necessary.

As output of USSI is often rather important, we have designed the program to occupy complete pages whatever type of line printer is used (72, 80, 135, ... character width printers; printer width is introduced via COMMON/PAGE/). This however implies the use of 2 and 4 byte INTEGER variables and variable formats which may reduce the portability of the program.

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** We will use in this paper the symbols used in program USSI although they often differ from usual conventions; for example, number average molecular weight is most of the time represented as $\bar{M}_N$ instead of AMWN.

Computer Physics Communications 15 (1978) 387–400
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# A NEW PROGRAM FOR CALCULATING MATRIX ELEMENTS OF ONE-PARTICLE OPERATORS IN *jj*-COUPLING

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Received 22 March 1978

## PROGRAM SUMMARY

*Title of program*: One-particle OPS in jj-coupling

*Catalogue number*: ACYM

*Computer*: IBM 360/195

*Installation*: Rutherford Laboratory, Chilton, Didcot, Oxfordshire, OX11 0QX, UK

*Operating system*: OS/360, Hasp

*Programming language used*: FORTRAN IV

*High speed storage required*: 80 kbytes (execution only)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes used*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1339

*CPC Library subprograms used*:

| *Catalogue number* | *Title* | *Ref in CPC* |
|---|---|---|
| AAHD | A NEW VERSION OF NJSYM | 8 (1974) 151 |
| ACRI | CFPJJ-CFP IN JJ-COUPLING | 4(1972)377 |
| ACRIOOOA | CORRECTION | 14(1978)311 |
| ACWE | MCP75 | 11(1976)397 |
| ACWEOOOA | CORRECTION | 14(1978)311 |

*References to other published version of this program*: Catalogue number: AAAD; Title: RDMEJJ; Ref. in CPC: 7 (1974) 225

*Keywords*: atomic, nuclear, multipole operators, open shells, *jj*-coupling

*Nature of the physical problem*
Calculation of the matrix elements of one-particle tensor operators occurring in atomic and nuclear theory between configuration state functions representing states containing any number of open shells in *jj*-coupling. The program calculates the angular part of these matrix elements.

*Method of solution*
The program is essentially a new version of RDMEJJ [1], written by J.J. Chang. The aims of this version are to eliminate inconsistencies from RDMEJJ, to modify its input requirements for consistency with MCP75 [2], and to modify its output so that it can be stored in a discfile for access by other compatible programs.

*Restrictions on the complexity of the problem*
The program assumes that the configurational states are built from a common orthonormal set of basis orbitals. The number of electrons in a shell having $j \geqslant 9/2$ is restricted to be not greater than 2 by the available CFP routines [3]. The present version allows up to 40 orbitals and 50 configurational states with $\leqslant 10$ open shells; these numbers can be changed by recompiling with modified COMMON/DIMENSION statements, The user should ensure that the CPC library subprograms AAGD, ACRI incorporate all current updates and have been converted to use double precision floating point arithmetic.

*References*

[1] J.J. Chang, Comput. Phys. Commun. 7 (1974) 225.
[2] I.P. Grant, Comput. Phys. Commun. 11 (1976) 397; 5 (1973) 263.
[3] I.P. Grant, Comput. Phys. Commun. 4 (1972) 377; 14 (1978) 311.

Computer Physics Communications 15 (1978) 401–415
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# I: A COMPUTER PROGRAM FOR NORMALIZATION AND INSTRUMENT CORRECTION OF NEUTRON DIFFRACTION DATA ON NON-CRYSTALLINE MATERIALS TO OBTAIN THE STATIC STRUCTURE FACTOR

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Received 14 March 1978

## PROGRAM SUMMARY

*Title of program*: FYINT

*Catalogue number*: ACYR

| *Computer*: | *Installation*: |
|---|---|
| IBM 370/168 | University of Missouri, Columbia, MO, USA |
| IBM 370/165 | NEUCC, Technical University of Denmark |

*Operating System*: 0S/VS2 4MVS

*Program language used*: FORTRAN

*High speed storage required*: 13 337 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, disk (2 files)

*No. of cards in combined program and test deck*: 1060

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACYS | FYPAR | 15 (1978) 417 |
| ACYT | PAR | 15 (1978) 431 |

*Keywords*: solid state, non-crystalline, neutron diffraction, structure factor, instrument correction, normalization, pair distribution, Fourier transform

*Nature of physical problem*
The structure factor of non-crystalline materials may be obtained from neutron diffraction data. After correction for background two important problems remain, namely a proper instrument correction and a normalization of the experimental data. With this program instrument corrections for samples with a cylindrical symmetry are calculated, and the data are normalized in a systematic way providing the structure factor for the material. The instrument corrections include corrections for attenuation of the neutron beam, incoherent scattering, multiple scattering and non-static behavior in terms of the Placzek correction. The normalization of the data is based on the macroscopic density of the sample.

*Method of solution* [1,2]
The multiple scattering is assumed to be isotropic and the calculation of the correction for non-static behavior is based on an approximate expression, where the specific interactions between atoms are not included. The validity of the expression is best for heavy elements and relatively small wave vector transfers. The data are normalized by a least squares fit calculation to the Fourier transform of the structure factor at small distances $r$, where it is given by the macroscopic density of the sample.

*Unusual features of the program*
The storage requirement depends on the number of experimental data and the number of neutron wave lengths used in

the experiment. In the present set up the storage requirement is set to 13 337 words, which are estimated to be satisfactory for a large number of cases.

*Restrictions on the complexity of the problem*
The calculation of multiple scattering and attenuation of the neutron beam is restricted to a cylindrical symmetry, and the data have to be corrected for background. The experiment should be performed in such a way as to make the Placzek correction as small as possible.

*References*

[1] F.Y. Hansen and K. Carneiro, Nucl. Instr. and Meth. 143 (1977) 569.
[2] F.Y. Hansen, T.S. Knudsen and K. Carneiro, J. Chem. Phys. 62 (1975) 1556.

Computer Physics Communications 15 (1978) 417–429
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# II. A COMPUTER PROGRAM FOR CALCULATION OF PARAMETERS NECESSARY FOR THE COMPUTATION OF RELIABLE PAIR DISTRIBUTION FUNCTIONS OF NON-CRYSTALLINE MATERIALS FROM LIMITED DIFFRACTION DATA

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Received 14 March 1978

## PROGRAM SUMMARY

*Title of program*: FYPAR

*Catalogue number*: ACYS

| *Computer*: | *Installation*: |
|---|---|
| IBM 370/168 | University of Missouri, Columbia, MO, USA |
| IBM 370/165 | NEUCC, Technical University of Denmark |

*Operating System*: 0S/VS2 4MVS

*Program language used*: FORTRAN

*High speed storage required*: 15 083 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line-printer, disk (1 file)

*No. of cards in combined program and test deck*: 482

*CPC library subprograms used*:

| *Cat. No.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACYR | FYINT | 15 (1978) 401 |
| ACYT | PAR | 15 (1978) 431 |

*Keywords*: solid state, non-crystalline, pair distribution function, structure factor, Fourier transform, truncation error

*Nature of physical problem*
The pair distribution function of non-crystalline materials may be obtained by a Fourier transform of the structure factor as calculated in part I [1] of this series. The structure factor is often limited in the sense that it shows significant oscillations at the maximal wave vector transfer obtainable. The Fourier transform of such functions, therefore, introduces truncation errors in the transformed function. With this program a parametrization of the small distance part of the pair distribution function is obtained according to a method described by us, which enables us to eliminate truncation error from the final pair distribution function. It is based on a least squares fit calculation of the small distance part of the pair distribution function obtained by a direct transform of the experimental structure factor and a model pair distribution function obtained from a model structure factor truncated at the same wave vector transfer as the experimental factor.

*Typical running time*
The running time depends on the number of structure factor data and the number of peaks in the least squares fit calculation. For the test example the running time is 8.2 s. The compilation time is included in this time, so if a compiled version of the program is used, the running time is reduced to 4.1 s.

*Unusual features of the program*
The storage requirement depends on the number of structure factor data and the number of peaks used to resolve the small distance part of the pair distribution function. In the present set-up the storage requirement is set to 15 083 words, which is estimated to be satisfactory for a large number of cases.

*Restrictions on the complexity of the problem*
The only restriction of the program is the high speed storage available.

*References*

[1] F.Y. Hansen, Comput. Phys. Commun. 15 (1978) 401.
[2] F.Y. Hansen, Comput. Phys. Commun. 15 (1978) 431.
[3] F.Y. Hansen and K. Carneiro, Nucl. Instr. and Meth. 143 (1977) 569.
[4] F.Y. Hansen, T.S. Knudsen and K. Carneiro, J. Chem. Phys. 62 (1975) 1556.

Computer Physics Communications 15 (1978) 431–435
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# III. A COMPUTER PROGRAM FOR CALCULATION OF RELIABLE PAIR DISTRIBUTION FUNCTIONS OF NON-CRYSTALLINE MATERIALS FROM LIMITED DIFFRACTION DATA

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Received 14 March 1978

## PROGRAM SUMMARY

*Title of program*: PAR

*Catalogue number*: ACYT

| *Computer*: | *Installation*: |
|---|---|
| IBM 370/168 | University of Missouri, Columbia, MO, USA, |
| IBM 370/165 | NEUCC, Technical University of Denmark |

*Operating System*: 0S/VS2 4MVS

*Program language used*: FORTRAN

*High speed storage required*: 8860 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line-printer, disk (1 file)

*No. of cards in combined program and test deck*: 124

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACYR | FYINT | 15 (1978) 401 |
| ACYS | FYPAR | 15 (1978) 417 |

*Keywords*: solid state, non-crystalline, pair distribution function, structure factor, truncation error

*Nature of physical problem*
This program calculates the final pair distribution function of non-crystalline materials on the basis of the experimental structure factor as calculated in part I [1] of this series and the parameters of the small distance part of the pair distribution function as calculated in part II [2] of this series. In this way, truncation errors may be eliminated from the final pair distribution function.

*Method of solution*
The calculations with this program depend on the results of calculations with the programs described in parts I and II of this series [1,2]. The final pair distribution function is calculated by a Fourier transform of a combination of an experimental structure factor and a model structure factor.

*Typical running time*
The running time depends on the number of data points in the structure factor and the number of data points in the final pair distribution function. For the test example, the running time is 1.4 s. The compilation time is included in this time, so if a compiled version of the program is used, the running time is reduced to 0.75 s.

*Unusual features of the program*
The storage requirement depends on the number of data points in the structure factor, the number of data points in the final pair distribution function and the number of peaks necessary to resolve the small distance part of the pair distribution function. In the present set-up a storage requirement is set to 8860 words which is estimated to be satisfactory for a large number of cases.

*Restrictions on the complexity of the problem*
The only restriction of the program is the high speed storage available.

*References*

[1] F.Y. Hansen, Comput. Phys. Commun. 15 (1978) 401.
[2] F.Y. Hansen, Comput. Phys. Commun. 15 (1978) 417.

Computer Physics Communications 15 (1978) 437–441
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# A PLOTTING PACKAGE FOR VISUALLY COMPARING THEORETICAL AND EXPERIMENTAL RESULTS

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Received 2 November 1977; in revised form 5 April 1978

## ADAPTATION SUMMARY

*Title of adaptation*: POLAR PLOT AND IMPROVEMENTS

*Adaptation number*: 0001

*Reference to original program*:
*Title of program*: APLOT;
*Catalog Number*: AAUN;
*Ref. in C.P.C.*: 9 (1975) 85

*Authors of original program*: J. Anderson, K.J.M. Moriarty and R.C. Beckwith

*High speed store required*: 18 kwords

*No. of bits in a word*: 60

*No. of cards required to effect adaptation (including directive cards)*: 1097

*Additional keywords*: polar graph

*Nature of physical problem*
Some shortcomings in our previous package, namely, no facility for polar plots, difficulties encountered when the data went outside the subject space and the absence of a dot–dashed line facility caused problems in implementing the package on a computer.

*Method of solution*
Using CalComp routines a polar plotting routine is developed. Improvements in the previous package for plotting linear–linear, log–linear and log–log graphs and histograms are also included.

*Restrictions on the complexity of the program*
The only restriction on the improved and extended package is the number of theoretical and experimental points to be plotted.

*Typical running time*
To generate figs. 1 to 4 of the present paper took about 9 s.

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## ERRATUM NOTICE

*Title of manuscript*: Calculation of wave-functions and collision matrix elements for one-electron diatomic molecules

*Author*: A. Salin

*Reference*: Comput. Phys. Commun. 14 (1978) 121

*Title of program*: GRAVE

*Catalogue number*: ACXX

Page 124 – eqs. (14a), (14b) and (14c) should be:

$$E_i(Z_1, R) = Z_1^2 E_i(1, RZ_1)\,, \tag{14a}$$

$$R_{ij}(Z_1, R) = Z_1 R_{ij}(1, RZ_1)\,, \tag{14b}$$

$$L_{ij}(Z_1, R) = L_{ij}(1, RZ_1)\,. \tag{14c}$$

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# ADAPTATION OF THE NEW VERSION OF THE REDUCED MATRIX ELEMENTS (AAKP) PROGRAM: INCLUSION OF THE CHECKING OF THE INPUT DATA *

K.M.S. SAXENA
*Division of Theoretical Chemistry, Department of Chemistry,*
*University of Alberta, Edmonton, Alberta, Canada T6G 2G2*

Received 10 April 1978

## ADAPTATION SUMMARY

*Title of the adaptation*: ADAPT TENSOR 2 TO CHECK DATA

*Adaptation number*: 0002

*Reference to the original program*:
*Title of the program*: Reduced Tensor Matrix Elements 2
*Catalog Number*: AAKP
*Ref. in C.P.C.*: 9 (1975) 370
*Authors of the program*: C.F. Fischer and K.M.S. Saxena

*Number of cards required to effect the adaptation (including the directive cards)*: 291

*CPC library subprograms used*: same as in the original program AAKP

*Additional keywords*: none

*Purpose of the adaptation*: checking of the input data for possible errors

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* This work has been supported in part by the National Research Council of Canada.

Computer Physics Communications 16 (1978) 65–71
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# AN INTEGRAL PACKAGE FOR ONE-CENTER INTEGRALS OVER SLATER-TRANSFORM-PREUSS FUNCTIONS

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Received 17 February 1978; in revised form 6 June 1978

## PROGRAM SUMMARY

*Title of program*: STP

*Catalogue number*: ACYU

*Computer*: TR 440; *Installation*: University of Bielefeld

*Operating system*: BS3

*Programming language used*: FORTRAN IV

*High speed storage required*: 32 000 words

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 673

*Keywords*: atomic physics, molecular physics, quantum chemistry, Slater–Transform–Preuss functions, one-electron integral, two-electron integral, theoretical methods, hypergeometric function

*Nature of physical problem*
One-center, one- and two-electron integrals over STP functions [1,2] are calculated to obtain the atomic wavefunctions to be used in quantum mechanical calculations.

*Method of solution*
The integrals are evaluated using special and general types of hypergeometric functions or a modified Gauss quadrature is employed.

*Restrictions on the complexity of the problem*
To include functions with angular quantum number higher than 2 the appropriate Condon–Shortley coefficients should be added.

*Typical running time*
Compilation time is 10 s, execution times depend on the types of functions used and the number of integrals calculated. A single-zeta type calculation of a second row atom including SCF iterations is 1 s.

*References*

[1] E. Yurtsever and D.D. Shillady, Chem. Phys. Lett. 40 (1976) 447; 43 (1976) 20.
[2] E. Yurtsever, Chem. Phys. 28 (1978) 243.

Computer Physics Communications 16 (1978) 73–83
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# CARS SPECTRAL PROFILES FOR HOMONUCLEAR DIATOMIC MOLECULES

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*Chemistry Division (Code 6110), Naval Research Laboratory, Washington, DC 20375, USA*

Received 24 April 1978

## PROGRAM SUMMARY

*Title of program*: CARS

*Catalogue number*: AAHJ

*Computer*: TI-ASC, IBM 360/75; *Installation*: Naval Research Laboratory, Washington, DC 20375

*Operating system*: 424

*Programming language used*: FORTRAN IV

*High speed storage required*: 50 000 words

*No. of bits in a word*: 32

*No. of magnetic tapes required*: none

*Other peripherals used*: Card reader, line printer

*No. of cards in combined program and test deck*: 749

*Keywords*: molecular physics, CARS, coherent anti-stokes Raman spectroscopy, Raman spectroscopy, spectroscopy, third-order susceptibility, nonlinear spectroscopy, four wave mixing, nonlinear optics, lasers, electrical discharge, plasma

*Nature of the physical problem*
Raman spectra of molecules can be obtained with a much higher degree of sensitivity using Coherent Anti-Stokes Raman Spectroscopy (CARS) [1]. Calculations based on comparisons of experimental CARS data with computer-synthesized spectra are very useful for the determination of temperature and molecular concentrations in many engineering and scientific applications. These calculations are also invaluable to the basic understanding of the CARS process itself. Some of these important applications include the study of combustion systems [2–5] and electrical discharges [6,7].

*Method of solution*
The program computes rotational and vibrational partition functions, populations, and the frequencies of all transitions allowed by selection rules for a given molecule under specified conditions. From these results and known spectroscopic constants [8], the square of the total third-order electric susceptibility [1,9], convoluted over a finite laser linewidth, is calculated as a function of frequency shift. This gives an adequate representation of the CARS spectral profile.

*Restrictions on the complexity of the problem*
The program currently performs calculations involving only homonuclear diatomic molecules. Straight forward modifications would be necessary if other types of molecules were to be considered. Furthermore, although the program can be used to calculate the O-, Q- and S-branches of the spectrum, it cannot calculate them simultaneously in an additive manner in its present form.

*References*

[1] W.M. Tolles, J.W. Nibler, J.R. McDonald and A.B. Harvey, Appl. Spectry. 31 (1977) 253; J.W. Nibler and G.V. Knighten, Topics in current physics (ed. A. Weber; Springer Verlag, Berlin, 1977) Ch. 7; A complete list of references may be found in these review articles.
[2] P.R. Regnier and J.P. Taran, Appl. Phys. Lett. 23 (1973) 240.

[3] P.R. Regnier, F. Moya and J.P. Taran, AIAA J. 12 (1974) 826.

[4] F. Moya, S.A.J. Druet and J.P. Taran, Opt. Commun. 13 (1975) 169.

[5] F. Moya, S. Druet, M. Pealat and J.P. Taran, AIAA Paper No. 76-29, presented at the AIAA 14th Aerospace Sciences Meeting, Washington, DC (January 26–30, 1976).

[6] J.W. Nibler, J.R. McDonald and A.B. Harvey, Opt. Comm. 18 (1976) 371.

[7] W.M. Shaub, J.W. Nibler and A.B. Harvey, J. Chem. Phys. 67 (1977) 1883.

[8] G. Herzberg, Molecular spectra and molecular structure, vol. 1, Spectra of diatomic molecules (Van Nostrand Reinhold Company, New York, 1950).

[9] R.N. De Witt, A.B. Harvey and W.M. Tolles, NRL Memorandum Report 3260, Naval Research Laboratory, Washington, DC 20375 (April 1976).

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# LIQUID DROP MODEL DEFORMATION ENERGIES OF NUCLEI WITH AXIAL SYMMETRY AND REFLECTION ASYMMETRY

D.N. POENARU, M. IVASCU
*Central Institute of Physics, P.O. Box 5222, R-76900, Magurele-Bucharest, Romania*

Received 21 March 1978; in final form 22 May 1978

## PROGRAM SUMMARY

*Title of program*: LIQUID DROP DEFORMATION ENERGIES

*Catalogue number*: ABQG

*Computer*: IBM 370/135; *Installation*: Central Institute of Physics

*Operating system*: DOS/VS-310

*Programming language used*: FORTRAN IV

*High speed storage required*: 33 kbyte

*Number of bits per byte*: 8

*Overlay structure*: none

*Other peripherals used*: card reader, line printer, card punch

*Number of cards in combined program and test deck*: 462

*Keywords*: low energy, nuclear physics, structure, liquid drop model, finite range, fission, fusion, heavy ion, collisions, Krappe–Nix integral, Coulomb energy, surface energy

*Nature of the physical problem*
The deformation dependent terms of the nuclear potential energy in the Myers–Swiatecki's liquid frop model [1] are: Coulomb and surface energies. For nuclear shapes with axial symmetry, they are expressed by two fold and simple integrals, respectively. The surface energy was redefined by Krappe and Nix [2] in order to take into account the finite range of nuclear forces. Calculation of this energy requires a three fold integration.

*Method of solution*
The multiple integrals involved are computed numerically by Gauss–Légendre quadrature. Because the nuclear shape is usually described by a different equation in the neck region, the accuracy and speed is improved by a suitable choice of four subintervals of integration.

*Restriction on the complexity of the problem*
The number of meshpoints for numerical quadrature are chose to assure the required accuracy for a given shape. Only yhe following values are allowed: $n = 4, 8, 12$ and $16$ for each of the four subintervals.

*Typical running time*
Typical running time on the IBM 370/135 for $n = 8$ and one deformation set is 12 s.

*Unusual features of the program*
The program as it stands is used for nuclear energies. But with few changes it may be used for calculating the electrostatic energy and the surface area of any body with axial symmetry and uniform distribution of matter and electric charge, assuming that the charge and matter density is a single-valued function of $Z$.

*References*

[1] W.D. Myers and W.J. Swiatecki, Nucl. Phys. 81 (1966) 1; Arkiv for Fysik 36 (1967) 343.
[2] H.J. Krappe and J.R. Nix, Proc. Symp. on Physics and chemistry of fission (IAEA, Vienna, 1974) vol. 1, p. 159.

Computer Physics Communications 16 (1978) 93–112
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# FOURIER ANALYSIS WITH SPLINES, A FORTRAN PROGRAM

C. POMPONIU* and M. SARARU
*Institute of Physics and Nuclear Engineering, P.O. Box 5206, Bucharest, Romania*

Received 10 May 1978

## PROGRAM SUMMARY

*Title of program*: TRIINT

*Catalogue number*: AAUX

*Computer*: IBM 370/135; *Installation*: Computing Office of the Institute of Physics and Nuclear Engineering, Bucharest

*Operating system*: DOS

*Programming language used*: FORTRAN IV

*High speed storage required*: 104 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 951

*Keywords*: general purpose, spline functions, Fourier analysis, Fourier coefficients, complex functions, approximation, interpolation

*Nature of physical problem*
There often arises the need for a good trigonometric representation of periodic continuous functions in various areas of physics and engineering. These functions can be given either by a formula or by their values at specified points. The subroutine package TRIINT provides a procedure for fast and accurate Fourier representation for functions of the former class because the discrete case can be treated in a similar way, once a suitable data-interpolation formula is found.

*Method of solution*
The analysed function is approximated first by a cubic spline interpolant, then the Fourier coefficients of the latter are constructed. Showing a rate of (asymptotic) decrease of $1/n^3$ these coefficients provide a good trigonometric approximation of the spline interpolant and of the analysed function itself in so far as the latter is well approximated by the spline interpolant.

*Restrictions on the complexity of the problem*
The main restrictions concern the dimensions of the arrays used in constructing the spline interpolant and in storing the computed coefficients for testing purposes. For more than 1800 knots the dimensions of ALFA (1800) in subroutine SPLINE and of all arrays in block /SPLTHT/ should be increased accordingly. The same holds true for the arrays in blocks /COEFF/ and /SERVCE/, if more then 501 Fourier coefficients are needed. To save high-speed storage, execution can be forced in single precision by punching C in the first column of all IMPLICIT REAL*8(A–H, O–Z) and FORTRAN-function defining cards.

*Typical running time*
The Central Processor Unit running time for computing 101 coefficients using a 127-knot spline interpolant was about 5s.

*Unusual features of the program*
The program was designed to work in stages in order that the user might control the accuracy of the computations as the program goes along, and pass to the next stage when the attained error level proves satisfactory.

*References*

[1] I.H. Ahlberg, E.N. Nilson and J.L. Walsh, The theory of splines and their applications, ch. 2 (Academic Press, New York, 1976).

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# A SUBROUTINE FOR APPROXIMATION BY CUBIC SPLINES IN THE LEAST SQUARES SENSE

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Received 12 June 1978

## PROGRAM SUMMARY

*Title of program*: BELLS

*Catalogue number*: AAPA

*Computer*: Hewlett-Packard 21 MX, type 2112A; *Installation*: Institute of Physics of the Charles University, Prague

*Operating system*: RTE-III

*Programming language used*: FORTRAN IV

*High speed core required*: ⩾26 kbyte

*Number of bits in a word*: 16

*Overlay structure*: none

*Number of tapes required*: none

*Other peripherals used*: card reader, line printer (HP digital plotter, optional)

*Number of cards in combined program and test deck*: 347

*Keywords*: general purpose, curve fitting, least squares, cubic splines

*Nature of the physical problem*
The subroutine computes the approximation to the experimental data points (not necessarily equidistant) by a sum of the cubic bell spline [1] functions in the least squares sense.

*Method of solution*
A system of linear equations with a band matrix is solved by Gaussian elimination

*Restriction on program complexity*
Present dimensions limit to 500 data points and the approximation up to 100 cubic splines, these limits may be changed by redimensioning

*Typical running time*
On the 21 MX computer the compilation takes about 70 s, while a typical 20 splines fit to 100 points takes about 5 s.

*Unusual features of the program*
1) The approximation can be found in an arbitrary interval ⟨XA, XB⟩ which is the part of ⟨X(1), X(NP)⟩ where X(1) and X(NP) are abscissae of the first and the last of the given experimental points. To a small extent (defined later) there is also a possibility to extrapolate beyond ⟨X(1), X(NP)⟩.
2) It is highly recommended to use the plotter for an immediate plotting of the result curve because there is no objective criterion for the determining of the optimum number of splines for the fitting. The right choice can be judged by knowing the physical nature of the problem, by the expected smoothness of the approximation, etc.

*References*
[1] P. Ciarlet, M.H. Schultz and R.S. Varga, Num. Math. 9 (1967) 394.

Computer Physics Communications 16 (1978) 119–127
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# INTERMEDIATE COUPLING COLLISION STRENGTHS FROM *LS* COUPLED *R*-MATRIX ELEMENTS

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Received 10 February 1978; in revised form 19 May 1978

## PROGRAM SUMMARY

*Title of program*: LSTOIC

*Catalogue number*: AAKY

*Computer*: IBM 370/168; *Installation*: The Pennsylvania State University, University Park, PA 16802 USA

*Operating system*: OS/360

*Programming language used*: FORTRAN IV

*High speed storage required*: 70 kwords

*No. of bits in a word*: 32

*No. of magnetic tapes required*: none

*Other preipherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1238

*Keywords*: atomic physics, electron–atom, scattering, fine structure transitions, intermediate coupling, *LS* coupling, collision strengths, mixing coefficients, *R*-matrix, Wigner coefficients, configuration mixing

*Nature of the physical problem*
Fine structure collision strengths for transitions between two groups of states in intermediate coupling and with inclusion of configuration mixing are obtained from *LS* coupled reactance matrix elements (*R*-matrix elements) and a set of mixing coefficients.

*Method of solution*
The *LS* coupled *R*-matrix elements are transformed to pair coupling, as described in ref. [1], using Wigner 6-*j* coefficients. From these pair coupled *R*-matrix elements together with a set of mixing coefficients, *R*-matrix elements are obtained which include the intermediate coupling and configuration mixing effects. Finally, from the latter *R*-matrix elements, collision strengths for fine structure transitions are computed (with inclusion of both intermediate coupling and configuration mixing).

*Restrictions on the complexity of the problem*
Array lengths may be adjusted to suit the user's needs and the available core storage. Only one $J_a$ and $J'_a$ value may be computed at a time.

*Typical running time*
The sample data comprising one energy, 2 initial states, 2 final states and 12 intermediate states took 16 s of computer system time of which 5 s was actual execution time.

*Unusual features of the program*
*LS* coupled collision strengths for transitions between energy terms are computed as a check on the input *R*-matrix data. The program also computes *LS* coupled collision strengths for transitions between fine structure levels to be compared with the calculated fine structure collision strengths which include both intermediate coupling and configuration mixing. It can do this from either pure configuration *LS* coupled *R*-matrix elements so that configuration mixing need not have been done separately, or it can instead use as input *LS* coupled *R*-matrix elements which already include configuration mixing. Of course, the set of mixing coefficients required as input in obtaining the final results for collision strengths for fine structure transitions with inclusion of both intermediate coupling and configuration mixing are different in the two cases. In the former one uses the *b* coefficients in eq. (111) of ref. [2], while in the latter case one uses the *f* coefficients in eq. (109) of ref. [2], as done in ref. [1].

Users are warned that arrays with more than three dimensions occur in the program.

*References*

[1] H.E. Saraph, Comput. Phys. Commun. 3 (1972) 256.
[2] M. Jones, Phil. Trans. Roy. Soc. 277A (1975) 587.

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Computer Physics Communications 16 (1978) 129–137
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# TRIP 1, A TIME-DEPENDENT RECOMBINATION IONISATION PACKAGE

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Received 27 January 1978; in revised form 26 June 1978

## PROGRAM SUMMARY

*Title of program*: TRIP 1

*Catalogue number*: ABUV

*Computer*: IBM 370/168; *Installation*: Kernforschungszentrum Karlsruhe

*Operating system*: MVS, JES3

*Programming language used*: FORTRAN

*High speed storage required*: 250 kwords

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 1412

*CPC Library subprograms used*:

| *Catalogue number*: | *Title*: | *Ref. in CPC*: |
|---|---|---|
| ABUJ | OLYMPUS | 9 (1975) 51 |

*Keywords*: atomic physics, ionisation, recombination, time-dependent, steady state, radiation, plasma, optically thin

*Nature of physical problem*

TRIP 1 has been constructed to follow the time-dependent ionisation and recombination processes in a plasma of any density. The program can be used by itself or together with hydrodynamic codes in any dimension.

*Method of solution*

To estimate the degree of ionisation in the plasma, we solve for the mean and mean square ionisation levels $\langle z \rangle$ and $\langle z^2 \rangle$. In general these are functions of electron density, temperature and time. Subsidiary variables are the radiation rates, internal energy, etc.

*Restrictions on the complexity of the problem*

In the present version of TRIP 1 we allow only for a single element plasma. The radiation transfer problem is avoided by assuming the plasma to be optically thin. Only the ground state population densities are considered and analytic expressions are used for the rate coefficients.

*Typical running time*

On the IBM 360/145 at Karlsruhe 100 timesteps with no iterations per timestep take 0.25 s.

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[*] Present address: Kommission der Europäischen Gemeinschaften, Europäisches Institut für Transurane, Postfach 2266, D-7500 Karlsruhe 1, Fed. Rep. Germany.

Computer Physics Communications 16 (1978) 139–146
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# RADIAL RADIATIVE FLUX IN CYLINDRICALLY SYMMETRIC ARCS

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Received 17 May 1978

## PROGRAM SUMMARY

*Title of program*: RADFL

*Catalogue number*: ABUW

*Computer*: CDC 7600; *Installation*: University of Manchester, Regional Computer Centre

*Operating system*: scope variation 2.1

*Programming language used*: FORTRAN IV

*High speed storage used*: 20 kwords

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined test deck*: 1038

*Keywords*: plasma physics, radiation flux, continuum, line, molecular band, cylindrical symmetry, nitrogen, electric arcs

*Nature of the physical problem*
In the core of high temperature cylindircal electric arcs a net radiative flux of energy occurs in the outward radial direction. The code described here calculates the radiative flux within a frequency range and at a radial position which are user-specified, taking account of continuum and line radiation and the $N_2$ (Birge–Hopfield no. 2) molecular band radiation. The spectral data used is for nitrogen.

*Method of solution*
The flux is evaluated by a combination of Simpson's and Trapezoidal formula for the triple definite integral from:

$$F(r_p) = -4 \int_{\upsilon_1}^{\upsilon_2} \int_0^{\pi} \int_0^{L} K'_\upsilon B_\upsilon G_1\Big(\int_0^{s} K'_\upsilon \mathrm{d}s\Big) \cos\emptyset \, \mathrm{d}\upsilon \, \mathrm{d}\emptyset \, \mathrm{d}s \,,$$

which is derived in the Long Write Up using the condition of cylindrical symmetry and the projected optical depth in the radial plane.

*Restriction*
The model assumes conditions for LTE are satisfied.

*Typical running time*
A frequency range covering 20–25 absorption coefficient maxima (lines or multiplets) takes about 170 s.

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* Now at: Mechanical Engineering Department, University of Nottingham, Nottingham N67 2RD, UK.

Computer Physics Communications 16 (1979) 175–179
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# FREINT, AN INTEGRATION ROUTINE CALCULATING FRESNEL DIFFRACTION

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Received 24 May 1978; in revised form 15 August 1978

## PROGRAM SUMMARY

*Title of program*: FREINT

*Catalogue number*: ACUB

*Computer*: Honeywell Bull 66/60

*Installation*: MPI Stuttgart

*Operating system*: GCOS

*Programming language used*: FORTRAN

*High speed store required*: 1591 words *

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 346

*Keywords*: optics, electron microscopy, Fresnel diffraction, integral transforms

*Nature of physical problem*
FREINT evaluates the integral

$$\int_{x_i}^{x_f} A(x) \exp(\mathrm{i}\, q(x' - x)^2)\, \mathrm{d}x \qquad [\mathrm{i} = (-1)^{1/2}]$$

occurring in optical transfer theory. By application of this integral the wave amplitude $A(t + d; x')$ at a plane $z = t + d$ can be calculated on some premises from the amplitude field $A(t; x)$, e.g. in electron microscopy if an object is imaged in a defocussed mode [1] (catch-word: Fresnel diffraction). $A(x)$ is given by a complex vector.

*Method of solution*
FREINT performs quadratic interpolation of the function $A(x)$ given by $N$ data points $(x_k, A_k)$ ($A_k$ complex) in any double interval $(x_k, x_{k+2})$, if $h_1 = x_{k+1} - x_k$ equals $h_u = x_{k+2} - x_{k+1}$. If not, linear interpolation is chosen. From the interpolatory coefficients the sub-integral values are calculated according to analytical rules and are added up to the final integral value.

*Restrictions on the complexity of the problem*
The integral transformation will be performed for any complex vector, the dimension $N$ of which is greater than or equal to 2 and is limited at the upper end only by limitations of storage. The parameter $q$ must not equal zero.

*Typical running time*
The execution times depend on $N$. On the Honeywell Bull 66/60 a vector of length 37 takes approximately 0.05 s, if the abscissae points are equally spaced.

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* For the present test version; 10 kwords including programs from system library.

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# LATTICE DYNAMICS OF ZINCBLENDE STRUCTURE COMPOUNDS USING DEFORMATION-DIPOLE MODEL AND RIGID ION MODEL

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Received 10 January 1978

*Title of program:* LATTICE DYNAMICS OF ZINCBLENDE

*Catalogue number*: ACMP

*Computer*: CDC Cyber 173, IBM 370/168; *Installation*: University of Aarhus, CNRS-CIRCE, Orsay

*Operating system*: CDC: Kronos Version 2.1.2-419-C3; IBM: OS-VS2, Release 3.7, JES 3 2.0.1

*Programming language used*: FORTRAN IV

*High speed store required*: 16 k (CDC), 89 k (IBM)

*No. of bits in a word*: 60 (CDC), 32 (IBM)

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: lineprinter

*No. of cards*: 1157

*Keywords*: solid state, semiconductor, lattice dynamics, phonons, dispersion curves, dynamical matrix, zincblende structure, diamond structure, deformation-dipole model, rigid ion model

*Nature of physical problem*
Determination of phonon dispersion and phonon eigenvectors for zincblende structure and diamond structure materials.

*Method of solution*
Deformation-Dipole model and Rigid ion model calculation of dynamical matrices (refs. [1–5])

*Restrictions on the complexity*
Zincblende structure (and diamond structure) crystals. Some compounds are not yet well described by the above models.

*References*

[1] M. Born and K. Huang, Dynamical theory of crystal lattices, (Oxford University Press, Oxford, 1954).
[2] A.A. Maradudin, E.W. Montroll, G.H. Weiss and I.P. Ipatova, Solid state physics, eds. H. Ehrenreich et al., Suppl. 3, 2nd ed. (Academic Press, New York and London, 1971).
[3] S.K. Sinha, CRC Crit. Rev. Solid State Sci. 3 (1973) 273.
[4] A.M. Karo and J.R. Hardy, Phys. Rev. 129 (1963) 2024; 141 (1966) 696; 181 (1969) 1272.
[5] K. Kunc, M. Balkanski and M. Nusimovici, Phys. Rev. B12 (1975) 4346.

Computer Physics Communications 16 (1979) 199–206
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# A CUBIC SPLINE INTERPOLATION OF UNEQUALLY SPACED DATA POINTS

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Received 3 May 1978; in revised form 8 September 1978

## PROGRAM SUMMARY

*Title of program*: CUSPLN

*Catalogue number*: ACYV

*Computer*: CDC 6600; *Installation*: University of London Computer Centre

*Operating system*: CDC Scope

*Programming language used*: FORTRAN IV

*High speed storage required*: 17.5 kwords

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: CalComp plotter

*No. of cards in combined program and test deck*: 828

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAUN | APLOT | 9 (1975) 85 |
| AAUN0001 | POLAR PLOT AND IMPROVEMENTS | 15 (1978) 437 |

*Keywords*: general purpose, interpolation, spline, cubic spline, natural cubic spline, curve length, differentiation, quadrature

*Nature of the physical problem*
Quite often an experiment results in a series of discrete data points in the interval $[x_0, x_N]$. The theorist then wishes to interpolate this data at some point $x \in [x_0, x_N]$ or at a large number of points covering the domain $[x_0, x_N]$ so that an interpolating curve may be drawn. The theorist may also wish to interpolate the discrete data points in order to i) calculate the length of the curve through the data points ii) calculate the area under the curve through the data points or iii) calculate the derivative of the curve through the data points over the domain $[x_0, x_N]$. The most efficient method of accomplishing this is with the cubic spline interpolation function [1].

*Method of solution*

The cubic spline interpolation function matrix equations are solved to give the second derivatives at the $N+1$ discrete data points. From these the cubic spline interpolation function equations in each interval $x \in [x_i, x_{i+1}]$ $(i = 0, 1, \ldots, N-1)$ are then constructed. The interpolation, or the first derivative of the interpolation, can then easily be carried out at the point $x \in [x_0, x_N]$.

*References*

[1] J.H. Ahlberg, E.N. Nilson and J.L. Walsh, The theory of splines and their applications (Academic Press, New York and London, 1967).

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# AN INVERSION OF QUANTUM MECHANICS

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Received 10 April 1977; in revised form 16 August 1978

## PROGRAM SUMMARY

*Title of programs*: MATRIXFORMAT, CLSSCLFORMAT

*Catalogue number*: ACYP

*Computer*: UNIVAC 1106; *Installation*: U. of Wisc.-Milwaukee Computer Services Division

*Operating system*: EXEC 8

*Programming language used*: FORTRAN

*High speed storage required*: 20 K

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, optional disc

*No. of cards in combined program and test deck*: 2563

*Keywords*: quantum correlations, quantum mechanics, probability, quantum model, matrix mechanics, social science, quantum psychology, density matrix, state and test matrices, quantum probabilities, mixed test, finite spin system, spin-system density matrix

*Nature of physical problem*
The task is to seek "quantum correlations" in raw probability data. A table of counts or probabilities is input to MATRIXFORMAT or to CLSSCLFORMAT. The first produces a quantum matrix model listing matrices and also trace-formula theoretical output probabilities; the second produces a classical model by being restricted to diagonal matrices. By comparing the relative success of these two programs in fitting the data, the user attempts to determine whether the data exhibit quantum interference phenomena, i.e., whether the data favor a quantum-mechanical interpretation. Another kind of application is determination of density matrices and test matrices from probability data in an already accepted quantum-mechanical context, without any prior assumption of a dynamical model.

*Method of solution*
A theory-experiment probabilty discrepancy function is directly minimized, starting from random states and tests. By changing an input "seed" integer for the pseudo-random number generator and re-executing, an independent random start is obtained, if an exploration for possible alternative local minima is desired.

*Restrictions on the complexity of the program*
$N \times N$ matrices, with $N = 2$, 3 or 4 in MATRIXFORMAT, $2 \leqslant N \leqslant 99$ in CLSSCLFORMAT. N is user-selected. Large values for the number of states ISTATE, of tests JTEST, or of outcomes of tests will need more memory, run longer, and output more profusely. The 36-bit word structure was not used in the logic; hence the program will probably run on installations with other word lengths.

*Typical running time*
$\approx 5 - \approx 15$ min. The longer time includes time for optimized compilation.

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# STATIC AND DYNAMIC MUONIC–ATOM CODES – MUON AND RURP *

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and

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Received 22 February 1978; in revised form 13 September 1978

## PROGRAM SUMMARY

*Title of program*: MUON

*Catalogue number*: ABNB

*Computers*: CDC 6400, 6600, 7600, IBM 370/168 double precision

*Installation*: Los Alamos Scientific Laboratory

*Operating system*: Any batch processor

*Programming language used*: ASA FORTRAN

*High speed storage required*: 25339 words as supplied, can vary

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer, card reader, card punch

*No. of cards in combined program, test deck and description*: 2382

*Keywords*: nuclear physics, spectroscopy, atomic physics, muonic atoms, energy levels, QED corrections

*Nature of physical problem*
Muonic-atom energy levels and wave functions are calculated. The results are corrected for nearly all important static effects, including finite nuclear size as produced by a user-specified nuclear charge distribution [1].

*Method of solution*
Fourth-order Runge–Kutta integration of the radial Dirac equations, with the secant method determining the eigenvalues. Corrections are either included as potentials in the Dirac equations or computed as first-order perturbations.

*Restrictions on the complexity of the system*
The code assumes spherical symmetry, so that effects of nuclear deformation may be treated only as static first-order perturbations. Dynamic muon–electron and muon–nuclear effects are neglected (the latter are calculated by RURP).

*Typical running times*
The code and test case as supplied are compiled, loaded, and executed in 59 s on a CDC-6600, of which 21 s is compilation time (FTN compiler with optimization level 2).

*Unusual features of the program*
The main arrays are allocated semi-dynamically in order to keep core requirements to a minimum. Although the code as supplied is set up for CDC computers, previous versions have been run successfully on IBM 370/168 using the H-compiler with the AUTODOUBLE option. Use of the code on low-precision machines is recommended only if extensive double precision is implemented.

---

* Work performed in part under the auspices of the United States AEC, ERDA, and DOE.

** Present address.

*Reference*

[1] extensive numerical results from this code are reported by G.A. Rinker and R.M. Steffen, At. Data and Nucl. Data Tables 20 (1977) 143.

## PROGRAM SUMMARY

*Title of program*: RURP

*Catalogue number*: ABNC

*Computers*: CDC 6400, 6600, 7600, IBM 370/168 double precision

*Installation*: Los Alamos Scientific Laboratory

*Operating system*: Any batch processor

*Programming language used*: ASA FORTRAN

*High speed storage required*: 44990 words as supplied, can vary

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer, card reader

*No. of cards in combined program, test deck and description*: 4564

*Keywords*: nuclear physics, spectroscopy, atomic physics, muonic atoms, nuclear polarization, dynamic hyperfine structure, energy levels, transition intensities

*Nature of physical problem*

Coupled muon–nuclear wave functions, energy levels, and transition energies and intensities are calculated. The results are corrected for nearly all effects of nuclear excitation [2–4].

*Method of solution*

The muon–nuclear Hamiltonian is represented in an angular-momentum basis and diagonalized to all order in a truncated subspace and to second order in the remainder of the infinite Hilbert space. The finite-space diagonalization is accomplished by standard means. The remaining diagonalization is accomplished by the implicit solution of the appropriate inhomogeneous differential equations in the muon radial coordinate using a band-matrix inversion technique.

*Restrictions on the complexity of the system*

No more than 9 muon levels and 8 nuclear levels may be included at any one time. The only magnetic interaction included is the static M1 HFS interaction.

*Typical running times*

The code and test cases as supplied are compiled, loaded and executed in 322 s on a CDC-6600, of which 43 s are compilation (FTN compiler with optimization level 2).

*Unusual features of the program*

The main arrays are allocated semi-dynamically in order to keep core requirements to a minimum. Although the code as supplied is set up for CDC computers, previous versions have been run successfully on IBM 370/168 using the H-compiler with the AUTODOUBLE option. Use of the code on low-precision machines is recommended only if extensive double precision is implemented.

*References*

[2] G.A. Rinker, Phys. Rev. A14 (1976) 18;
[3] G.A. Rinker and J. Speth, Nucl. Phys. A 306 (1978) 360.
[4] G.A. Rinker and J. Speth, Nucl. Phys. A 306 (1978) 397.

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Computer Physics Communications 16 (1979) 243–265
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# ALFVEN – A TWO-DIMENSIONAL CODE BASED ON SHASTA, SOLVING THE RADIATIVE, DIFFUSIVE MHD EQUATIONS

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and

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*Naval Research Laboratory, Washington DC, USA*

Received 23 May 1978

## PROGRAM SUMMARY

*Title of program*: ALFVEN

*Catalogue number*: ABUX

| *Computer* | *Installation* |
|---|---|
| CDC 6500 | ACCU, Utrecht |
| CDC 6600 | Computer Centre, Groningen |
| IBM 370/168 | CECAM, Orsay, France |
| IBM 370/158 | CRI, Leiden |

*Operating system*: SCOPE 3.4 resp. OS-MVT or OS-MVS

*Program language used*: FORTRAN IV

*High speed storage required*: 55 kwords (CDC), 300 kbytes (IBM)

*No. of bits in a word*: 60 (CDC), 32 (IBM), single precision

*Overlay structure*: none

*No. of magnetic tapes*: none

*Other peripherials used*: card reader, line printer, magnetic disks

*No. of cards in combined program and test deck*: 2600

*Keywords*: Diffusive, radiative MHD, 2-dim, second-order accuracy, explicit convection, implicit diffusion, monotonic solutions, SHASTA numerical scheme, low-diffusion scheme

*Nature of physical problem*
A two-dimensional computer program to be used for solving hydrodynamic and hydromagnetic equations in various geometries [1,2]. The effects of gravity, ohmic dissipation and -diffusion, radiative losses and thermal conduction are include through an implicit, time-split coupled, step. The convective part of the equations is solved by the SHASTA numerical cod [3–7], having second-order accuracy but guaranteeing monotonicity in the directly-convected quantities. One-dimensional and isothermal applications are possible.
The program uses the equation for conservation of total energy ($U$-version).

*Method of solution*
Vectorized, two-dimensional explicit convection step with predictor–corrector ordening for second-order solution with removal of numerically produced extrema, time-split coupled to an implicit, tridiagonal matrix solver for physical conduction, radiation and diffusion [8].

---

* Presently at The Auroral Observatory, PB 953, 9001 Tromsö, Norway.

*Typical running time*
Achieving equilibrium in longest physical time scale will require typically 1200 time steps. Duration of one time step (−5% for adiabatic, −25% for diffusion free calculations): 22 s (CDC 6500), 6 s (CDC 6600), 4 s (IBM 370/168), 15 s (IBM 370/158) for a 63 × 43 grid in single precision.

*References*

[1] K.V. Roberts and D.E. Potter, Magnetohydrodynamic calculations, in Methods in computational physics, vol. 9, eds. Alder, Fernbach and Rotenberg (Academic Press, New York, London, 1970) p. 339.
[2] W.J. Weber, Thesis, University of Utrecht (1978).
[3] J.P. Boris and D.L. Book, J. Comput. Phys. 11 (1973) 38.
[4] J.P. Boris, SHAS2D – A fully compressible hydrodynamics code in 2 dimensions, NRL Memorandum Report 2542, Washington (1972).
[5] D.L. Book, J.P. Boris and K. Hain, J. Comput. Phys. 18 (1975) 248.
[6] J.P. Boris and D.L. Book, J. Comput. Phys. 20 (1976) 397.
[7] J.P. Boris, Flux-corrected transport modules for solving generalized continuity equations, NRL Memorandum Report 3237, Washington (1976).
[8] S.I. Braginskii, Rev. Plasma Phys. 1, Consultants Bureau, New York (1965).

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Computer Physics Communications 16 (1979) 267–271
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# NUMERICAL EVALUATION OF GEOMAGNETIC DYNAMO INTEGRALS (ELSASSER AND ADAMS–GAUNT INTEGRALS)

Wooil MOON *

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Received 3 April 1978; in revised form 4 September 1978

## PROGRAM SUMMARY

*Title of program*: ELSGAU

*Catalogue no.*: ACYX

*Computer*: IBM 370/158

*Installation*: Newfoundland and Labrador Computing Services Ltd.

*Operating system*: OS

*Program language used*: FORTRAN IV

*High speed storage required*: 25 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 354

*Keywords*: geophysics, Elsasser integral, Adams–Gaunt integral, geomagnetic dynamo integrals

*Nature of physical problem*
Numerical evaluation of Elsasser integrals and Adams–Gaunt integrals [1] to apply to the normal mode studies of realistic earth models.

*Method of solution*
Elsasser and Adams–Gaunt integrals are expanded using 3-*J* vector coupling coefficients [2] and numerically computed checking appropriate selection rules.

*Restrictions on the complexity of the problem*
As long as the order and degree of the integrands are integers there is no restriction.

*Typical running time*
0.36 s for the test run.

*References*

[1] D.E. Winch, J. Geomagn. Feoelec. 26 (1974) 87.
[2] K. Srinivasa Rao and K. Venkatesh, New FORTRAN programs for angular momentum coefficients, Comput. Phys. Commun. 15 (1978) 227.

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Computer Physics Communications 16 (1979) 273–280
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# AN INTERPOLATION METHOD FOR DATA SETS WITH JUMP DISCONTINUITIES

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Received 3 April 1978; in revised form 4 September 1978

## PROGRAM SUMMARY

*Title of program*: JMPDIS

*Catalogue number*: ACYW

*Computer*: IBM 370/158

*Installation*: Newfoundland and Labrador Computing Services Ltd.

*Operating system*: OS

*Program language used*: FORTRAN IV

*High speed storage required*: 60 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No of tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 477

*Keywords*: interpolation, cubic Hermite polynomial basis functions, jump discontinuity, cubic spline

*Nature of problem*
Any spatial or temporal data set with sharp jump discontinuities may be interpolated by this subroutine JMPDIS. The data set can have a finite number of discontinuities (less than 10 in this case) or no discontinuity at all.

*Method of solution*
All interpolation calculations for data sets with jump discontinuities are done using cubic Hermite polynomial basis function. Smooth data sets will be interpolated by cubic spline method when the number of discontinuities in the input data is zero.

*Restrictions on the complexity of the problem*
The number of input data points and the desired output are limited by DIMENSION statements which can be changed by the user. The number of allowed jump discontinuities is 10 but this can also be changed.

*Typical running time*
0.9 CPU for the test run.

*References*

[1] M.H. Schulz, Spline analysis (Prentice Hall, London, Englewood Cliffs, 1973) p. 24.

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Computer Physics Communications 16 (1979) 285–299
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# I. GENERATOR OF DETERMINANTAL NON-RELATIVISTIC ATOMIC STATES FROM SPECTROSCOPIC NOTATION, COMPUTATION OF MATRIX ELEMENTS

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Received 9 January 1978; in revised form 4 October 1978

## PROGRAM SUMMARY

*Title of program*: TERM

*Catalogue number*: AAKU

*Computer*: UNIVAC 1110; *Installation*: Université d'Orsay, France

*Operating system*: UNIVAC 1110 EXEC 8

*Program language used*: FORTRAN V

*High speed storage required*: 50 000 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: 1 (for output)

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 7994

*Keywords*: atomic structure, angular momentum, spectroscopic notation, coupling, determinantal states, angular matrix element, reduced matrix element, W operators, creation operator, annihilation operator, coefficients of fractional parentage quasispin, Slater integrals, hyperfine structure operators, multipole operators, $n$-particle operators

*Nature of the physical problem*

The program generates the decomposition of an atomic state into Slater determinants from its description in the usual spectroscopic notation. The output is directly usable by the program EXCGH [1]. The program can also compute matrix elements and reduced matrix elements of operators $\tilde{a}$, $a^+$, $a^{(1/2}$ $\Sigma_{i<j \ldots <k}\, w_i^{(1)} w_i^{(1')} \ldots w_j^{(2)} w_j^{(2')} \ldots w_k^{(n)}$ as well as products of such operators coupled in any way. The results are given in an exact $a\sqrt{b}/c\sqrt{d}$ form.

*Method of solution*

Each shell is generated by the projection method. Couplings are computed from $3jm$ coefficients. Matrix elements are calculated from determinantal states.

*Restrictions on the complexity of the problem*

Each shell is given in $SL$ coupling. There are no restrictions for further coupling between shells and operators.

*Typical running time*

The test run containing 16 computations takes 19 s. In general, computation of determinantal states is fast, but computation of matrix elements can be very long.

*Unusual features of the program*

FORTRAN V instructions INCLUDE and PARAMETER, intrinsic functions FLD, ENCODE and DECODE.

*References*

[1] J.J. Labarthe, Comput. Phys. Commun. 16 (1979).

Computer Physics Communications 16 (1979) 301–309
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# II. GENERATOR OF ATOMIC EXCITED TERMS FROM ANGULAR CONSIDERATIONS

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Received 9 January 1978; in revised form 4 October 1978

## PROGRAM SUMMARY

*Title of program*: EXCGH

*Catalogue number*: AAKV

*Computer*: UNIVAC 1110; *Installation*: Université d'Orsay, France

*Operating system*: UNIVAC 1110 EXEC 8

*Program language used*: FORTRAN V,

*High speed storage required*: 46 000 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: 2 (for output)

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 4048

*CPC Library subprogram used (for data)*: Cat. No.: AAKU; *Title*: TERM; *Ref. in CPC*: 17 (1979) 000.

*Keywords*: atomic structure, excitations, angular, configuration interaction, multiconfigurational Hartree–Fock, MCHF, energy matrix, Slater integrals, specific isotope shift, hyperfine structure, spin–orbit, dipole, second order, Slater determinants, Russell–Saunders

*Nature of the physical problem*
The program generates the excited terms adapted to the computation of 2nd order values of the operators $H$ (energy), $\Sigma$ (specific isotope shift), hyperfine structure ($sC^2$, $C^2$, $l$, $s$), spin–orbit and dipole $C^1$. It computes the angular part of the energy matrix and various operators and edits the results in a form suitable for Froese-Fischer's multiconfigurational Hartree–Fock program [1].

*Method of solution*
Determinantal states of given $M_S$ and $M_L$ values are used. Angular matrix elements are computed from the $c^k(lm, l'm')$ coefficients [2]. In each excited configuration the basis formed of Slater determinants is reduced to a minimum number of states contributing to the 2nd order.

*Restrictions on the complexity of the problem*
$nl$ shell with $l \leq 5$.

*Typical running time*
For case 1 of test run 0.9 s, including the computation of the $c^k$ coefficients. For case 2 of test run 0.1 s.

*Unusual features of the program*
FORTRAN V instructions INCLUDE and PARAMETER, intrinsic functions FLD and DECODE.

*References*

[1] C. Froese-Fischer, Comput. Phys. Commun. 1 (1969) 151; 14 (1978) 145.
[2] E.U. Condon and G.H. Shortley, The theory of atomic spectra (Cambridge University Press, 1963) p. 175.

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# III. ANALYTIC APPROXIMATIONS OF RADIAL ORBITALS FOR MULTICONFIGURATIONAL HARTREE–FOCK COMPUTATIONS

J.J. LABARTHE
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Received 9 January 1978; in revised form 4 October 1978

## PROGRAM SUMMARY

*Title of program*: EDD

*Catalogue number*: AAKW

*Operating system*: UNIVAC 1110 EXEC 8

*Program language used*: FORTRAN V

*High speed storage required*: 52 000 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: 3 (for output)

*Other peripherals used*: card reader, line printer, card puncher (option)

*No. of cards in combined program and test deck*: 7087

*CPC Library subprogram used (for data)*: *Cat. No.* AAKV; *Title*: EXCGH; *Ref. in CPC*: 17 (1979) 000

*Keywords*: atomic structure, non relativistic, excitations, virtual orbital, analytic, configuration interaction, multiconfigurational Hartree–Fock, MCHF, Slater functions, nonorthogonality, central field integral, energy, specific isotope shift, second order, crossed second order, simplex method

*Nature of the physical problem*
An analytic non-relativistic atomic multiconfigurational variational program.

Central field integrals and non-orthogonality between orbitals are accepted. The program makes it possible easily to determine approximate excited orbitals in order to have initial values for the numerical multiconfigurational (MCHF) program [1]. All necessary input for ref. [1] is written in file 9.

*Method of solution*
The various orbitals can be described numerically, analytically or developed on basis orbitals (numerical orbitals or Slater functions). The various parameters are determined to minimize the energy or the 2nd order energy by a 2-loop simplex method (inner loop for development coefficients, outer loop for exponents).

*Restrictions on the complexity of the problem*
*nl* shells with $l \leqslant 5$; excited configurations must be obtained from configuration 1 by bi- or monoexcitations; non-orthogonality between orbitals must be such that in the expression of energy the most complicated overlaps are of the type $(nl/n'l)(n_1l'/n_2l')$ with $l \neq l'$.

*Typical running time*
For determining one orbital to a good precision, the necessary time is 1–2 min.

*Unusual features of the program*
FORTRAN V instructions INCLUDE, PARAMETER, intrinsi functions FLD and DECODE. A required diagonalisation subroutine is not included in the deck.

*Reference*

[1] C. Froese-Fischer, Comput. Phys. Commun. 1 (1969) 151
14 (1978) 145.

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# IV. APPROXIMATION OF NUMERICAL ORBITALS BY SLATER FUNCTIONS

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Received 9 January 1978; in revised form 4 October 1978

## ADAPTION SUMMARY

*Title of adaptation*: QFO

*Adaptation number*: 0001

*Reference to original program*: *Cat. No.:* AAKW; *title:* EDD; *ref. in Comput. Phys. Commun. 16 (1979) 311.*
*Author of original program*: J.J. Labarthe

*Computer*: UNIVAC 1110; *Installation*: Université d'Orsay, France

*Operating system*: UNIVAC 1110 EXEC 8

*Programme language used*: FORTRAN V

*High speed storage required*: 49 000 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: 2 (for output)

*Other peripherals used*: card reader, line printer, card puncher (option)

*No. of cards in combined adaptation and test deck*: 1071

*Keywords*: atomic structure, non-relativistic, orbital, Slater functions, simplex method

*Nature of the physical problem*
Non relativistic atomic orbitals given in a numerical form, as obtained from the multiconfigurational Hartree–Fock program [1] are approximated by Slater functions. This permits initial values to be obtained for analytic configuration interaction programs, like for example ref. [2].

*Method of solution*
The projection of the numerical orbitals on the Slater functions is maximised by the simplex method.

*Restrictions on the complexity of the problem*
$nl$ shells with $l \leqslant 5$.

*Typical running time*
1 min

*References*

[1] C. Froese-Fischer, Comput. Phys. Commun. 1 (1969) 151.
[2] A. Hibbert, Comput. Phys. Commun. 9 (1975) 141.

Computer Physics Communications 16 (1979) 331–343
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# A COMPUTER PROGRAM FOR INTEGRALS OF MOTION

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Received 4 January 1978; in revised form 4 October 1978

## PROGRAM SUMMARY

*Title of program*: COSTANTI DEL MOTO

*Catalogue number*: ACYO

*Computer*: UNIVAC 1106; *Installation*: Centro di Calcolo dell' Università, Milano, Italy

*Operating system*: UNIVAC 1106 EXEC 8

*Program language*: FORTRAN

*High speed storage required*: 42 000 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: Card reader, line printer, card punch

*No. of cards in combined program and test deck*: 800

*Keywords*: astrophysics, celestial mechanics, classical mechanics, stellar systems, integrals of motion

*Nature of physical problem*
The classical problem of constructing formal integrals for a Hamiltonian of harmonic oscillators coupled by polynomial interactions is considered.

*Method of solution*
An algorithm recently proposed [1] is applied which allows very fast computation of the integrals.

*Restrictions on the complexity of the problem*
The restrictions, imposed by array dimensions, are described in detail in the long write up, section 3.6.

*Typical running time*
The computation of one integral up to order 8 for a model with 2 degrees of freedom required an execution time of about 25 s on the UNIVAC 1106.

*Reference*
[1] A. Giorgilli and L. Galgani, Cel. Mech. 17 (1978) 267.

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# WORKER, A PROGRAM FOR HISTOGRAM MANIPULATION

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*Los Alamos Scientific Laboratory, Los Alamos, NM 87545, USA*
*and*
*University of Texas, Austin, USA*

Received 22 December 1976; in revised form 5 May 1978

## PROGRAM SUMMARY

*Title of program*: WORKER

*Catalogue number*: ABPH

*Computer*: PDP-11/45 with floating point processor; *Installation*: Los Alamos Meson Physics Facility, Los Alamos, New Mexico

*Operating system*: RSX-11D version 6

*Program language used*: FORTRAN-IV PLUS

*High-speed storage required*: a recommended minimum of 80 kwords total for operating system and user memory partitions

*No. of bits in a word*: 16

*Overlay structure*: overlaid

*No. of magnetic tapes required*: none

*Other peripherals used*: disk, display terminal such as a Tektronix Model 4010

*Number of card images in combined program and test deck*: 10 000

*Key words*: general purpose, utility, data manipulation, histogram, display, output, calculator

*Nature of physical problem*
A set of programs is provided which may link to any user-written program, permitting dynamic creation of histograms as well as display, manipulation and transfer of histogrammed data. With wide flexibility, constants within the user's code may be set or monitored at any time during execution.

*Method of solution*
The user's code needs only to generate data and request its entry into a histogram. Histograms are dynamically created outside the user's task space. These histograms may be displayed and manipulated by WORKER. An on-line compiler in WORKER accepts mathematical statements very similar to FORTRAN and permits manipulation of up to 240 variables which are made available to the user's program through a Shareable, Global Memory Area.

*Restriction on the complexity of the problem*
A maximum of 40 histograms may be allocated in memory; however, the amount of core used by these histograms may be any amount of memory remaining after the required task images are loaded. As many as 8 histograms can be combined, displayed, or transferred to a disk data file, on a channel-by-channel basis, in virtually any mathematical combination which includes functions such as SQRT, MAX, MIN as well as the standard operators +, –, *, / and **.

*Typical running time*
The amount of time required to store the user's data into a histogram is approximately 150 $\mu$s. The time required for display of a histogram or its transfer to the disk is a few seconds depending upon the size of the histogram. The time required to compile and to generate the necessary task images is done with a batch job which takes roughly 35 min but need only be done once.

*Unusual features of the program*
The programs provided are designed specifically for a multi-task space environment in which communication between tasks can be achieved easily and efficiently. The reference to HSTMGE in this paper is provided as an example and the user must provide his own, machine dependent histogramming

package which can then be coupled to WORKER, using RSX. Users are warned that WORKER is installation dependent in its present form.

Computer Physics Communications 16 (1979) 363–372
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# A SET OF SUBROUTINES FOR SIMULATION OF ELECTRON–PHOTON CASCADES

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Received 3 January 1978; in revised form 10 July 1978

## PROGRAM SUMMARY

*Title of program*: EMCASR

*Catalogue number*: AAUV

*Computer*: EC 1020, EC 10 series, IBM 360/, IBM 370;
*Installation*: INRNE, Sofia

*Operating system*: EC Disk Operating System

*Programming language used*: FORTRAN IV

*High speed storage required*: 3437 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: none

*No. of cards in combined program and test deck*: 730

*Keywords*: high energy physics, cosmic rays, electron–photon cascade, bremsstrahlung, pair production, Compton effect, Coulomb scattering, Monte Carlo simulation, composition, rejection

*Nature of physical problem*
This set of subroutines can serve as a basis for Monte Carlo programs simulating electron–photon cascades.

*Method of solution*
Every subroutine uses Monte Carlo techniques to simulate one of the following processes: bremsstrahlung, pair production, Compton effect, multiple Coulomb scattering. The subroutine DIST calculates the free path realized in the interaction.

*Restrictions on the complexity of the problem*
The subroutines are designed for energies corresponding to screening parameter $\gamma < 2$. Versions of bremsstrahlung and pair production programs for full screening are also included. This means that the energy range is from several MeV to $10^{11}$ MeV for air. In heavier media the energy interval is narrower because of the lack of validity of the Born approximation around the lower limit and the influence of the Landau–Pomerantchuk effect for the upper one.

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Computer Physics Communications 16 (1979) 373–381
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# CALCULATIONS OF GENERALIZED HARMONIC OSCILLATOR BRACKETS

J. DOBEŠ

*Institute of Nuclear Physics, Czechoslovak Academy of Sciences,*
*CS 250 68 Řež, Czechoslovakia*

Received 7 August 1978

## PROGRAM SUMMARY

*Title of program*: TAMOBR

*Catalogue number*: ABGR

| *Computer*: | *Installation*: |
|---|---|
| IBM 370/135 | Institute of Information, Theory and Automation, Prague |
| EC 1040 | Nuclear Research Institute, Řež |

*Operating system*: OS/VS1, OS/ES

*Programming language used*: FORTRAN IV

*High speed storage required*: 16 896 words

*Number of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader and line printer

*Number of cards in combined program and test deck*: 609

*Keywords*: nuclear, nuclear structure, nuclear reaction, shell model, two-body operator matrix elements, Talmi–Moshinsky bracket, generalized harmonic oscillator bracket, harmonic oscillator

*Nature of the physical problem*
The generalized harmonic oscillator brackets [1] form the transformation matrix for the transition from the single-particle coordinates to the centre of mass and relative coordinates in a two-particle harmonic oscillator basis. Unequal masses of particles are considered.

*Method of solution*
Recently published closed form for oscillator bracket [2] is used. Two subprograms are presented, one for the evaluation of a single bracket, the other for simultaneous calculation of a set of brackets with fixed angular momenta.

*Restrictions of the complexity of the problem*
Restrictions are given by the size of the core storage assigned to dimensioned quantities. The present version allows the computation of oscillator brackets with $\max(l, L, l_1, l_2) = 13$ and $\max(n + N, n_1 + n_2) = 32$.

*Typical running time*
Roughly 100 brackets per second on the IBM 370/135 computer

*Unusual features of the program*
Double precision REAL∗8 arithmetic is used on computers with 32 bit words.

*References*

[1] M. Moshinsky, Nucl. Phys. 13 (1959) 104; Yu.F. Smirnov, Nucl. Phys. 39 (1961) 346.
[2] J. Dobeš, J. Phys. A10 (1977) 2053.

Computer Physics Communications 16 (1979) 383–387
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# ON NUMERICAL BESSEL TRANSFORMATION

B. SOMMER and J.G. ZABOLITZKY
*Institut für Theoretische Physik, Ruhr-Universität, Bochum, Fed. Rep. Germany*

Received 15 August 1978

## PROGRAM SUMMARY

*Title of program*: FTRANS

*Catalogue number*: ACZC

*Computer*: CDC 7600; *Installation*: University Köln, Fed. Rep. Germany

*Operating system*: Scope 3.4.4

*Program language used*: FORTRAN

*High speed storage required*: 7000 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 396

*Keywords*: general purpose, Fourier transform, Bessel transform, spherical Bessel function, Filon integration, numerical integration

*Nature of physical problem*
We present a computer program to calculate the three dimensional Fourier or Bessel transforms and definite integrals with Bessel functions.

Numerical integration of systems containing Bessel functions occurs in many physical problems, e.g. electromagnetic form factor of nuclei, all transitions involving multipole expansions at high momenta.

*Method of solution*
Filon's integration rule is extended to spherical Bessel functions. The numerical error is of the order of the Simpson error term of the function which has to be transformed. Thus one gets a stable integral even at large arguments of the transformed function.

*Typical running time*
The test run compiled in 1.37 s and executed in 0.45 s on the CDC 7600.

Computer Physics Communications 16 (1979) 389–393
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# A NEW VERSION OF PIRK (ELASTIC PION–NUCLEUS SCATTERING) TO HANDLE DIFFERING PROTON AND NEUTRON RADII *

H.O. FUNSTEN
*Physics Department, College of William and Mary, Williamsburg, VA 23185, USA*

Received 1 May 1978; in revised form 10 November 1978

## PROGRAM SUMMARY

*Title of program*: PIRK 2

*Catalogue number*: AAWC

*Computer*: IBM 370/158; *Installation*: William and Mary, Williamsburg, VA 23185

*Operating system*: SVS

*Programming language used*: Fortran IV, Compiler G

*High speed core required*: 124 kbyte

*No. of bits per byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 822

*Reference to other published version of this program*: Cat. No.: ABCJ; Title: PIRK; Comput. Phys. Commun. 8 (1974) 130.

*Keywords*: nuclear, high energy, pion, elastic scattering, angular distribution, optical model, Klein-Gordon, complex potential, phase shift, cross section, separate n, p densities.

*Nature of physical problem*
This program is a modification of the Eisenstein–Miller program [1] for calculating elastic pion–nucleus differential cross sections using free $\pi$–N scattering amplitudes.

*Purpose of the revision*
This revision permits the use of separate proton and neutron radii for the nuclear density function $\rho(r)$.

*Typical running time*
CPU time of approximately 15 s was used for the test run.

*Reference*

[1] R.A. Eisenstein and G.A. Miller, Comput. Phys. Commun. 8 (1974) 130.

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* This work is supported by a grant from the National Science Foundation.

Computer Physics Communications 16 (1979) 395–400
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# A NEW VERSION OF DWPI (INELASTIC PION–NUCLEUS SCATTERING) TO INCORPORATE MICROSCOPIC FORM FACTORS AND DIFFERING PROTON AND NEUTRON RADII *

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Received 1 May 1978; in revised form 10 November 1978

## PROGRAM SUMMARY

*Title of the program*: DWPI 2

*Catalogue number*: AAWD

*Computer*: IBM 370/158; *Installation*: William and Mary, Williamsburg, VA 23185

*Operating system*: SVS

*Programming language used*: FORTRAN IV, Compiler G

*High speed core required*: 236 kbyte

*No. of bits per byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1090

*CPC library subprograms used*: Cat. No.: AAWC; Title: PIRK 2; Comput. Phys. Commun. 16 (1979) 389.

*Reference to other published version of this program*: Cat. No.: ABIG; Title: DWPI; Comput. Phys. Commun. 11 (1976) 95.

*Keywords*: nuclear, high energy, pion, inelastic scattering, distorted wave, impulse approximation, optical model, angular distribution, Klein–Gordon, cross section, microscopic form factor, reduced matrix element.

*Nature of physical problem*
This is a modification of the Eisenstein–Miller program [1] for calculation of collective inelastic pion–nucleus differential cross sections using free $\pi$–N scattering amplitudes.

*Purpose of the revision*
This revision permits the additional use of microscopic (shell model) proton and neutron form factors. It also incorporates separate proton and neutron radii for the nuclear density $\rho(r)$ generating the distorted wave optical potential.

*Typical running time*
CPU time of approximately 4 min was used for the test run.

*Reference*
[1] R.A. Eisenstein and G.A. Miller, Comput. Phys. Commun. 11 (1976) 95.

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* Thir work supported by a grant from the National Science Foundation.

Computer Physics Communications 17 (1979) 239–282
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# FORSIM VI: A PROGRAM PACKAGE FOR THE AUTOMATED SOLUTION OF ARBITRARILY DEFINED DIFFERENTIAL EQUATIONS

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*Chalk River, Ontario K0J 1J0, Canada*

Received 27 July 1978; in revised form 15 November 1978

## PROGRAM SUMMARY

*Title of program*: FORSIM VI

*Catalogue number*: ACYZ

*Computer*: CDC 175 or 6600; *Installation*: Chalk River Nuclear Laboratories, Atomic Energy of Canada Ltd., Chalk River, Ontario K0J 1J0, Canada *

*Operating system*: CDC NOS/BE

*Programming language used*: FORTRAN IV

*High speed storage required*: $100_8$ kwords minimum

*No. of bits in a word*: 60

*Overlay structure*: CDC overlay

*No. of magnetic tapes required*: none

*Other peripherals used*: disc files, card reader, line printer

*No. of cards in combined program and test deck*: 6985

*Reference to other published version of this program*: previous program version, AAICA 3 (1975) 195.

*Keywords*: general purpose, partial differential equations, ordinary differential equations, integration, method of lines, differential quadrature

*Nature of the physical problem*
Mathematical models comprising partial and ordinary differential equations arise in many scientific disciplines. A large class of these models may be automatically transformed into initial value problems involving only coupled ordinary differential equations, which may then be solved numerically by error-controlled integration. The FORSIM package solves a set of user-defined equations in this manner. These may be ordinary differential equations, and/or partial differential equations in up to three dimensions.

*Method of solution*
The user describes his equations and related conditions in a single FORTRAN subroutine, according to certain clearly defined rules. This subroutine may call other routines if necessary.

Any partial differential equations are then transformed into ordinary differential equations in time, using locally one-dimensional piecewise approximation formulae in the spatial dimensions. Boundary conditions are incorporated in the approximation formulae. The resulting ordinary differential equations are integrated by algorithms which choose the optimal step size to maintain the estimated local truncation error below a specifiable tolerable value. The definition of the equations and the type and frequency of sampling printout are entirely within the user control; the transformation and integration are performed automatically, but the user may exert optional controls governing these operations.

*Restrictions on the complexity of the problem*
The program is implemented to accept a maximum of 1000 ordinary differential equations, but this limit may be readily changed in a simple user written routine. The main restriction is upon the spatial system, which should have a regular boun-

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* The program will work on any CDC 6000 or 170 series computer and may be converted to other similar size computers without major difficulty.

dary, but may be any orthogonal coordinate system providing the equations are written in a compatible form.

*Typical running time*
Running time is a complicated function of the number of differential equations, the integration option used, the behaviour of the equations and the requested accuracy.

*Unusual features of the program*
The integration routines in FORSIM have been intensively developed and tested. They include an option to accelerate predictor corrector convergence by an automatic sparse matrix assessment of the system Jacobian, and the application of the error criterion is also unique. The transformation of partial differential equations into ordinary differential equations for two and three dimensions is analogous to the simple one-dimensional case. A user's manual complete with bibliography, background theory, programming philosophy and applications examples is available [1], and is in fact essential, as the range of possible application is too immense to give anything but an overview here.

*References*

[1] M.B. Carver, D.G. Stewart, J.M. Blair and W.N. Selander, Atomic Energy of Canada Limited report AECL-5821 (February 1978).

Computer Physics Communications 17 (1979) 283–300
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# DE VOGELAERE'S METHOD WITH AUTOMATIC ERROR CONTROL

John P. COLEMAN and Julie MOHAMED
*Department of Mathematics, University of Durham, South Road, Durham, UK*

Received 18 August 1978

## PROGRAM SUMMARY

*Title of program*: RADISH

*Catalogue number*: ACZB

*Computer*: IBM 370; *Installation*: NUMAC (Northumbrian Universities Multiple Access Computer)

*Operating system*: MTS

*Programming language*: FORTRAN IV

*High speed storage required*: 2686 words (DEVOG 1043)

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes*: none

*Other peripherals*: card reader, line printer

*Number of cards in combined program and test deck*: 604

*Keywords*: general purpose, de Vogelaere's method, Schrödinger equation, error control, numerical solution, phase shifts, second-order differential equation, integration

*Nature of the physical problem*
The subroutine DEVOG solves any equation of the form $y'' = f(x, y)$. The test program, which provides an example of this subroutine in operation, solves the single-channel Schrödinger equation for scattering of an electron by the static potential of atomic hydrogen, for a specified energy $E$ and angular momentum $L$, and calculates the scattering phase shift.

*Method of calculation*
The differential equation is solved by de Vogelaere's method [1] and the local truncation error is controlled by using the results of Coleman and Mohamed [2]. To calculate the phase shift the numerical solution in the asymptotic region is expressed as a linear combination of spherical Bessel functions.

*Restrictions on the complexity of the problem*
The subroutine DEVOG is applicable to any linear or nonlinear equation of the form $y'' = f(x, y)$. The restriction of the test program to the static potential of hydrogen may be removed by changing the function subprogram F. The test program requires $L \leqslant 4$ but this restriction is easily removed (see section 5.1).

*Running time*
The test run which accompanies this paper took 3.4 s CPU time, in a time-sharing environment, to calculate 27 phase shifts. (A separate compilation-only run took 2.1 s.)

*Unusual features*
The steplengths used in solving the differential equation are chosen automatically by the program in accordance with a local accuracy criterion supplied by the user.

*References*

[1] R. de Vogelaere, J. Res. Nat. Bur. Std. B 54 (1955) 119.
[2] J.P. Coleman and J. Mohamed, Math. Comput. 32 (1978) 751.

Computer Physics Communications 17 (1979) 301–304
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# COUNTING A SMALL NUMBER OF RADIOACTIVE ATOMS, SECOND PROGRAM

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Received 6 September 1978

## PROGRAM SUMMARY

*Title of program*: Counting few radioactive atoms/2

*Catalogue number*: AAUY

*Computer*: UNIVAC 1108; *Installation*: State Computer Centre, Helsinki

*Operating system*: EXEC-8

*Programming language used*: FORTRAN

*High speed storage required*: 25326 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader and line printer

*No. of cards in combined program and test deck*: 144

*Reference to other published version of this program*: *Cat. No.* AAUS; *Title*: Counting few radioactive atoms; *Ref. in CPC*: 13 (1977) 281

*Keywords*: nuclear physics, radioactive decay, radioactive atoms, small samples, decays, statistical analysis, Bayesian analysis

*Nature of physical problem*
Determination of the posterior probability $P(n)$ that a small sample of a radioactive isotope contained $n$ atoms at the end of production, when the counts in the subsequent counting periods are known.

*Method of solution*
The modified method explained in section 2.3 of ref. [1].

*Restriction on the complexity of the problem*
$n \leqslant 129$.

*Typical running time*
108 s (95 s CPU) on UNIVAC 1108.

*Unusual features of the program*
Bayesian methods utilizing prior information, as explained in ref. [1].

*Reference*

[1] A.M. Aurela, Comput. Phys. Commun. 13 (1977) 281.

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# EXTENSION TO HIGH FREQUENCIES OF A PROGRAM FOR CALCULATING THE ANGULAR DISTRIBUTION OF NONRELATIVISTIC BREMSSTRAHLUNG

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Received 13 October 1978

## ADAPTATION SUMMARY

*Title of adaptation*: BREMSSTRAHLUNG INTENSITY 2

*Adaptation number*: 0001

*Reference to original program*:
*Cat. No.*: ACYJ; *Title*: BREMSSTRAHLUNG INTENSITY (NR); *Ref. in CPC*: 15 (1978) 125

*Authors of original program*: Alicia Bañuelos and Félix Rodríguez-Trelles

*No. of cards required to effect adaptation*: 245

*Additional keywords*: high frequency X-rays, short-wave limit

*Nature of physical problem*
The applicability of the existing program is extended to the high frequency range of emission.

*Method of solution*
The total intensity $I_t$ (integrated over all the angles of observation $\phi$) is calculated by Weinstock's series expansions [1,2]. Fast convergent series [3,4] are used to evaluate one polarisation component ($I_y = I_z$), whereby the other one ($I_x$) and the angular distribution $I(\phi)$ are obtained. In order to reduce the computing time, near the critical energy ratio ($R = h\nu/U \approx R_0 \approx 0.97$) intensities are obtained by interpolation.

*Restrictions on the complexity of the problem*
The only restrictions arise from the error in the values of the physical constants [5]. Electron energies below $0.0001 Z^2$ keV may result in an underflow condition.

*Typical running time*
Running times range between ≈1 s for moderate electron energy values and ratios ($E = U/Z^2 = 0.001$ to 100 keV; $R = 0.01$ to 0.85), and up to 40 s near the critical ratio $R_0$, with EPS = $10^{-20}$.

*References*
[1] R. Weinstock, Phys. Rev. 61 (1942) 584.
[2] R. Weinstock, Phys. Rev. 64 (1943) 276.
[3] A. Bañuelos and F. Rodríguez-Trelles, J. Phys. B 11 (1978) 1663.
[4] A. Bañuelos and F. Rodríguez-Trelles, Comput. Phys. Commun. 15 (1978) 125.
[5] Particle Data Group, Rev. Mod. Phys. 48 (1976) S35.

Computer Physics Communications 17 (1979) 309–316
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# A FORTRAN PROGRAM TO INTERPRET PULSED FIELD-GRADIENT SPIN-ECHO DIFFUSION DATA

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Received 15 November 1978

## PROGRAM SUMMARY

*Title of program*: DIFFUS2

*Catalogue number*: ABNE

*Computer*: IBM 370/158; *Installation*: The University of Akron, Akron, OH 44325, USA

*Operating system:* 0S/MVS

*Programming language used*: FORTRAN IV (G1)

*High-speed store required*: 10 000 words (40 kbt) exclusive of loader

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, 132-column line printer

*Number of cards in combined program and test deck*: 781

*Keywords*: Diffusion, nuclear magnetic resonance, spin echo, pulsed magnetic field gradient method, steady gradient method, polymer science, chemistry

*Nature of physical problem*
NMR spin echo attenuation of the diffusing species, caused by steady and pulsed magnetic field gradients, is interpreted in terms of diffusion constants.

*Method of solution*
Various least-squares techniques are used to find the diffusion constant, and optionally, the constant spin echo of a non-diffusing species and to detect deviations from the model. Comprehensive error analysis and plot are provided.

*Restrictions on program complexity*
The present limit of 40 data points is easily extended.

*Typical running time*
On the IBM 370/158 III, the program compiles (G1 compiler) in about 6 s CPU; a single case with full analysis takes slightly over 1 s CPU.

*Unusual features of the program*
(1) Three or more data points (spin echo height ± error vs. field gradient pulse length) are required for a least-squares determination of diffusion coefficient;
(2) arbitrary diffusing nuclear species, steady and pulsed field gradients, and rf and gradient pulse timings are accommodated;
(3) non-diffusing nuclear species can be accounted for, and true multicomponent diffusion and restricted diffusion can be detected;
(4) a full error analysis coupled with chi-square considerations provides uncertainties of all derived parameters and checks the applicability of the selected model. A plot of data and fit is provided on the line printer.

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# APPLICATION OF THE GENERALIZED BACKWARD SUBSTITUTION METHOD TO SOLVE A CLASS OF LINEAR SYSTEMS

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Received 27 June 1978; in revised form 7 September 1978

## PROGRAM SUMMARY

*Title of program*: APICS

*Catalogue number*: ACZJ

*Computer*: C.D.C. 7326; *Installation*: Ecole Polytechnique Fédérale de Lausanne, Suisse

*Operating system*: N.O.S. B.E.

*Programming language used*: FORTRAN IV

*High speed core required*: 3800 words

*Number of bits in a word*: 60

*Overlay structure*: none

*Other peripherals used*: disc

*Number of cards in combined program and test deck*: 235

*Keywords*: general purpose, matrix, backward substitution, band matrices, linear systems

*Nature of physical problem*
General purpose subprogram solving linear systems corresponding to tridiagonal matrices in which the elements are replaced by submatrices. As an example, one can mention the discretized form (in time and space) of very general parabolic equations. A stable numerical scheme leads to such a system of linear equations [1].

*Method of solution*
Generalization to matrices of the backward substitution method [2].

*Restriction on the complexity of the problem*
All the submatrices have the same dimensions.

*Typical running time*
The running time depends on two parameters:
*n*: dimension of submatrices
*I*: number of submatrices along the diagonal
For example:

| *n* | *I* | Time of CPU |
|---|---|---|
| 10 | 5 | 0.940 |
| 5 | 10 | 0.438 |
| 10 | 10 | 2.079 |
| 5 | 20 | 0.964 |
| 20 | 5 | 5.468 |

*Unusual features of the program*
The same problem might be solved by some classical methods, but the proposed method allows us to leave out all the zeroes of the matrix and to save memory and CPU time.

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# ACCURATE BESSEL FUNCTIONS $J_n(z)$, $Y_n(z)$, $H_n^{(1)}(z)$ AND $H_n^{(2)}(z)$ OF INTEGER ORDER AND COMPLEX ARGUMENT *

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*Englefield Green, Egham, Surrey TW20 0EX, UK*

Received 6 June 1978; in revised form 15 January 1979

## PROGRAM SUMMARY

*Title of program*: BESJYH

*Catalogue number*: ACYQ

*Computer*: CDC 6600, CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: CDC NOS/BE, SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: 6 kwords (BESJYH: 3043, CJ: 498, CY: 883, CH: 1112)

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 1521

*Keywords*: general purpose, atomic, molecular, nuclear, expansion, representation, eikonal, impact parameter, helicity, partial wave, Bessel functions, Kelvin functions, Neumann functions, Weber's function, Hankel functions, complex functions

*Nature of physical problem*
The Bessel function appears in a wide range of physical applications, and in particular where there is axial symmetry. The package contains complex function routines to calculate $J_n(z)$, $Y_n(z)$, $H_n^{(1)}(z)$ and $H_n^{(2)}(z)$ for integer $n$ and complex $z$.

*Method of solution*
The method of solution is based on the ascending series representations and asymptotic forms of the Bessel functions $J_n(z)$ and $Y_n(z)$ and asymptotic forms of the modified Bessel functions $I_n(z)$ and $K_n(z)$; all of these are given in ref. [1].

*Restrictions on the complexity of the problem*
The program will return results for all values of $|z|$ up to machine overflows in the Bessel functions. The size of the order should not be too large (say, $|n| \leqslant 15$) or accuracy will be lost. For large $|n|$, the user should incorporate into the program the formulae given in ref. [1] for Debye's asymptotic expansions or better, the uniform asymptotic expansions. The value of the relative accuracy parameter, EPS, should not be set below about $10^{-11}$. For the asymptotic region, the accuracy EPS may not always be achieved (since the asymptotic series may have to be truncated at their lower terms), in which case the output parameter ISET will indicate this and an estimation of the relative error is also produced. The functions $Y_n(z)$, $H_n^{(1)}(z)$ and $H_n^{(2)}(z)$ have a branch point at the origin, together with a cut along the negative real axis.

*Typical running time*
The test run output at the end of the Long Write Up took about 4.2 s.

*References*

[1] M. Abramowitz and I.A. Stegun, Handbook of mathematical functions with formulas, graphs and mathematical tables (Dover Publications, New York, 1968).

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* Part of the Royal Holloway College Special Functions Mathematics Project.

Computer Physics Communications 17 (1979) 337–343
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# SLIT HEIGHT SMEARING CORRECTION IN SMALL ANGLE X-RAY SCATTERING
## I: INTENSITY CORRECTION PROGRAM *

Moshe DEUTSCH
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Received 6 June 1978

## PROGRAM SUMMARY

*Title of program*: CORECTEX

*Catalogue number*: AASB

*Computer*: IBM 370/168; *Installation*: Bar-Ilan University Computer Center, Ramat-Gan, Israel

*Operating system*: OS/VS2

*Programming language used*: FORTRAN IV G

*High speed storage required*: 47 000 words

*No. of bits in a word*: 32

*Overlay structure*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1761

*CPC library subprograms used (for data)*: *Cat. No.*: AASC; *Title*: FFITEX; *Ref. in CPC*: 17 (1979) 345

*Keywords*: crystallography, X-ray, scattering, diffraction, smearing, slit

*Nature of the physical problem*
The use of pinhole collimators in small angle X-ray scattering is impractical due to the low intensity obtained at the detector. Instead, long narrow slits, or their equivalents are used to collimate the beam. Consequently the measured intensity is an integral of the intensity scattered through a range of angles rather than the intensity scattered at the nominal measured angle [1]. This effect is known as the slit-height smearing effect.

To obtain the ideal intensity scattered at a unique angle, as if pinhole collimation was feasible, the data must be corrected for this effect. The present program is an implementation of our exact solution to this problem [2,3]. It yields highly accurate results as discussed in ref. [2].

*Method of solution*
Each corrected intensity value is obtained by integrating an expression involving the measured data and a correction function $g(t)$. This function is the solution of an integral equation involving the slit transmission function $f(t)$ [2]. A method was developed for solving this equation exactly using Laplace transform techniques, and the solutions for a large number of different forms of $f(t)$ are given in refs. [3,4].

Prior to using this program, the following preparatory procedure is required. First, the transmission function $f(t)$ of the apparatus to be used in the experiment must be measured. Then, an appropriate form of $f(t)$ is chosen from ref. [3] or [4] and fitted to the data using another program [5]. The parameters obtained in the fit automatically define the $g$-function to be used for correcting the scattering intensity data measured with the same apparatus. These parameters and the measured intensity values serve as input to the present program. Note that the data fitting procedure need be performed only once for a given apparatus.

*Restrictions on the complexity of the problem*
Only 250 intensity values can be corrected by the present version in a single run.

*Typical running time*
About 50 s for 250 intensity values.

*References*
[1] A. Guinier and G. Fournet, Small angle scattering of X-rays (John Wiley, New York, 1955).
[2] M. Deutsch and M. Luban, J. Appl. Cryst. 11 (1978) 87.
[3] M. Luban and M. Deutsch, (1979) to be published.
[4] M. Deutsch and M. Luban, International Union of Crystallography, Supplementary Publication No. SUP 32945 (1978); copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.
[5] M. Deutsch, Comput. Phys. Commun. 17 (1979) 345.

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* This work was supported by a grant from the United States–Israel Binational Science Foundation (BSF), Jerusalem, Israel.

Computer Physics Communications 17 (1979) 345–349
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# SLIT HEIGHT SMEARING CORRECTION IN SMALL ANGLE X-RAY SCATTERING II: COMPUTATION OF THE CORRECTION FUNCTION *

Moshe DEUTSCH
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Received 6 June 1978

## PROGRAM SUMMARY

*Title of program*: FFITEX

*Catalogue number*: AASC

*Computer*: IBM 370/168; *Installation*: Bar-Ilan University Computer Center, Ramat-Gan, Israel

*Operating system*: OS/VS2

*Programming language used*: FORTRAN IV G

*High speed storage required*: 8 500 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes used*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 584

*Keywords*: crystallography, X-ray, scattering, diffraction, smearing, slit, small-angle

*Nature of the physical problem*
The author's exact solution of the slit height smearing problem in small angle X-ray scattering [1–3] and its implementation [4], require the use of a correction function $g(t)$ in the correction formula. The parameters defining this function are obtained by fitting an appropriate analytic form to the measured values of the transmission function $f(t)$ of the slit system used in the scattering experiment. The present program performs the required fit and calculates the fit parameters.

*Method of solution*
The fit is done by minimizing the sum of the squares of the differences between the measured transmission function values, and the values of the parametrized analytic function. The method used is a version of the variable metric method [5] which does not require linear search [6], and consequently is very fast. The output of the program is the set of fit parameters.

*Restrictions on the complexity of the problem*
Only 200 measured values of the slit height transmission function can be handled by the present version.

*Typical running time*
About 1.4 s for 140 transmission function values.

*References*
[1] M. Deutsch and M. Luban, J. Appl. Cryst. 11 (1978) 87.
[2] M. Luban and M. Deutsch, (1979) to be published.
[3] M. Deutsch and M. Luban, International Union of Crystallography, Supplementary Publication No. SUP32945 (1978), copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1 NZ, England.
[4] M. Deutsch, Comput. Phys. Commun. 17 (1979) 337.
[5] W.C. Davidon, Argonne Nat. Lab. report ANL-5990 Rev. (1959); R. Fletcher and M.J.D. Powell, Comput. J. 6 (1963) 163.
[6] R. Fletcher, Comput. J. 13 (1970) 317.

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* This work was supported by a grant from the United States–Israel Binational Science Foundation (BSF), Jerusalem, Israel.

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Computer Physics Communications 17 (1979) 351–355
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# COULOMB FUNCTIONS WITH COMPLEX ANGULAR MOMENTA

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and

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Received 17 October 1978

## PROGRAM SUMMARY

*Title of program*: CCOULM

*Catalogue number*: ABND

*Computer*: CDC 6600; *Installation*: University of Texas Computer Center

*Operating system*: UT-2

*Programming language used*: FORTRAN IV

*High speed storage required*: 10816 words

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 400

*Keywords*: general purpose, nuclear, atomic, Schrödinger, scattering, reactions, Regge, complex angular momentum, wave function, Coulomb, complex Coulomb, potential, asymptotic expansion, phase shift, logarithm of complex gamma function

*Nature of physical problem*
The subroutine CCOULM calculates regular and irregular Coulomb functions and their derivatives associated with complex angular momenta. This program may thus be used, for example, in locating Regge poles that appear in atomic and nuclear scattering problems [1].

*Method of solution*
The calculation utilizes the asymptotic expansion method of Fröberg [2]. When the asymptotic expansion does not give a satisfactory result at a desired $\rho$, a larger value is chosen for $\rho$ and the differential equation is solved inward for the irregular solution. Then the method of Wills [3] is used to obtain the regular solution. The complex Coulomb phase shift is obtained by using a subroutine which calculates the logarithm of the gamma function for complex argument.

*Restrictions on the complexity of the problem*
Subroutine CCOULM can be used for real values $\rho$ and $\eta$ and for complex (as well as real) angular momentum $l$ that satisfy the condition $\eta^2 << \rho$ and $|l|^2 << \rho$. Even when this condition is not fulfilled, the program may be used with somewhat reduced accuracy.

*Typical running time*
The evaluation of regular and irregular Coulomb wave functions and their derivatives for a given value of $l$ takes about 0.3 s of the CDC 6600 computer.

*References*

[1] T. Tamura and H.H. Wolter, Phys. Rev. C6 (1972) 1976; T. Takemasa and T. Tamura, ibid., C18 (1978) 282.
[2] C.E. Fröberg, Rev. Mod. Phys. 27 (1955) 399.
[3] J.G. Wills, J. Comput. Phys. 8 (1971) 162.

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* On leave from Department of Physics, University of Saga, Saga 840, Japan.

** Supported in part by the U.S. Department of Energy.

Computer Physics Communications 17 (1979) 357–364
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# A BICUBIC SPLINE INTERPOLATION OF UNEQUALLY SPACED DATA

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and

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Received 30 August 1978; in revised form 10 January 1979

## PROGRAM SUMMARY

*Title of program*: BISPLIN

*Catalogue number*: ACZG

*Computer*: CDC 6600; *Installation*: University of London Computer Centre

*Operating System*: CDC SCOPE

*Programming Language used*: FORTRAN IV

*High speed storage required*: 5.4 kwords

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter

*No. of cards in combined program and test deck*: 749

*Keywords*: general purpose, interpolation, spline, bicubic spline, best approximation, de Boor's method

*Nature of physical problem*
A theorist may wish to interpolate data known to be a function of two variables. Often the data are not known on a regular grid, but are distributed irregularly. The "best approximation" when interpolating data which can be assumed to be error free is with the bicubic spline method [1,2].

*Method of solution*
We use de Boor's method and one dimensional cubic spline interpolation to calculate the coefficients of the spline in the rectangle $[x_i, x_{i+1}] \times [y_j, y_{j+1}]$. We can then obtain an interpolated value for the function and its first derivatives.

*Restrictions on the complexity of the problem*
The number of $x$-data points must be less than 25 and the number of $y$-data points must be less than 10. These values can be changed by the user. The point $(x, y)$ at which an interpolated value for the function is required must always lie in the rectangle $[x_1, x_n] \times [y_1, y_m]$. The program makes no restrictions on the spacing of the data points on the $x$ and $y$ axes.

*Typical running time*
The test run output took about 4.4 s.

*References*

[1] J.H. Alberg, E.N. Nilson and J.L. Walsh, The theory of splines and their applications (Academic Press, New York and London, 1967).
[2] C.A. Micchelli and T.J. Rivlin, Optional estimation approximation theory (Plenum Press, New York, 1977).

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Computer Physics Communications 17 (1979) 365–374
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# AN INTEGRAL EQUATION PROGRAM TO CALCULATE RADIAL WAVE FUNCTIONS AND SCATTERING PHASE SHIFTS OF SHORT-RANGE LOCAL INTERACTIONS

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Received 11 October 1978; in revised form 16 January 1979

## PROGRAM SUMMARY

*Title of program*: SCHRODINTEQN

*Catalogue number*: AAIE

*Computer*: ICL 1906S; *Installation*: University of Sheffield

*Operating system*: GEORGE 4

*Programming language used*: FORTRAN IV

*High speed storage required*: 27 kwords

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter

*No. of cards in combined program and test deck*: 374

*Keywords*: Schrödinger equation, quantum mechanical scattering, atomic scattering, nuclear scattering, molecular scattering, wave function, phase shift, local interaction, central potential, integral equation

*Nature of physical problem*
Determination of radial wave functions and scattering phase shifts of short-range local interactions for any value of the orbital angular momentum $l$ (= 0, 1, 2, 3, ...) over any (user) specified range of positive energies.

*Method of solution*
Quadrature solution of partial-wave Schrödinger integral equation.

*Restrictions on program complexity*
Present maximum of 100 quadrature points can be increased by altering two cards. Local interaction must be of the form

$$V(r) = \sum_t A_t \exp(-\mu_t r)/r + \sum_t B_t \exp(-\rho_t r)\,,$$

but the program can be easily modified to handle other short-range central potentials.

*Typical running time*
To set up and solve the equations of the method with $n$ quadrature points, per energy value (using optimizing FORTRAN compiler on ICL 1906S):

| $l$ | Approximate time (s) | | |
|---|---|---|---|
| | $n = 20$ | $n = 40$ | $n = 50$ |
| 0 | 0.1 | 0.6 | 1.1 |
| 1 | 0.2 | 0.8 | 1.4 |
| 2 | 0.2 | 1.1 | 1.8 |
| 3 | 0.3 | 1.2 | 1.9 |

*Unusual features of the program*
Program is in single precision form. Users of computers with short wordlengths are advised to convert the program to double precision form.

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# A PROGRAM FOR SOLVING SYSTEMS OF HOMOGENEOUS LINEAR INEQUALITIES

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*CERN, Geneva, Switzerland*

Received 7 November 1978; in revised form 18 January 1979

## PROGRAM SUMMARY

*Title of program*: LIHOIN

*Catalogue number*: ACZH

*Computer*: CDC 7600; *Installation*: CERN, Geneva

*Operating system*: CDC scope

*Programming languages used*: FORTRAN IV

*High speed store required*: 720 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 556

*Keywords*: general purpose, linear inequalities, Fourier expansion, positive functions, polyhedral cones, matrix, scattering amplitude, unitarity

*Nature of the physical problem*
The unitarity condition for physical scattering amplitudes implies the positivity of the imaginary parts of the partial waves. In an explicit construction of amplitudes this leads to inequality constraints for certain expansions.

*Method of solution*
The Motzkin–Burger rules are used to obtain iteratively the solution polyhedral cone of a system of homogeneous linear inequalities.

*Restrictions on the complexity of the problem*
It is assumed that the matrix of the system is of rank $N$, the number of unknowns. Similar to ill-conditioned systems of linear equations, a system of inequalities may also be ill-conditioned, and the program may fail in such cases. Note also that the number of intermediate vectors can become very large, and that some systems are inconsistent.

*Running time*
The running time is difficult to estimate. It depends not only on the dimensions of the system matrix, but also on its elements.

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* On leave of absence from Universität Kaiserslautern, Fed. Rep. of Germany. Supported in part by the Deutsche Forschungsgemeinschaft.

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# SIPSOL – A SUITE OF SUBPROGRAMS FOR THE SOLUTION OF THE LINEAR EQUATIONS ARISING FROM ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS

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Received 13 October 1978; in revised form 2 February 1979

## PROGRAM SUMMARY

*Title of program*: SIPSOL

*Catalogue number*: ACZL

*Computer*: CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: SCOPE 2.1.4

*Programming language used*: FORTRAN

*High speed storage*: $10N + C$ words, where $N$ = number of mesh points and $C \approx 1000$

*Number of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1021

*Keywords*: general purpose, Stone's algorithm, strongly implicit procedure, iterative, elliptic, partial, differential equations

*Nature of physical problem*
SIPSOL is a suite of subprograms for iteratively inverting a set of linear equations obtained from the discretisation of an arbitrary elliptic partial differential equation over a rectangular grid of mesh points.

*Method of solution*
A strongly implicit procedure using Stone's algorithm [1].

*Restrictions on the complexity of the problem*
In this version the mesh must be rectangular, although arbitrary boundary conditions may be specified. A five point difference operator must be used, giving a sparse five diagonal matrix system. The mesh may be non-uniform. A subprogram is supplied for calculating iteration parameters for the method, these are calculated for the general anisotropic diffusion equation; as a function of the mesh, or as a scalar.

*Typical running time*
For a mesh of 1024 points, a reduction in the L2 residual norm of 6 orders of magnitude can be obtained in 0.2–1.0 s on a CDC 7600.

*Unusual features of the program*
The surface output routine LIST in the test procedure uses A10 format (CDC 7600).

*Reference*

[1] H.L. Stone, Siam J.Numer. Anal. 5 (1968) 530.

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# ADAPTATION: NUMERICAL SOLUTION OF THE KRAMERS–KRONIG TRANSFORMS BY TRAPEZOIDAL SUMMATION AS COMPARED TO A FOURIER METHOD

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Received 19 July 1978; in revised form 20 January 1979

## ADAPTATION SUMMARY

*Title of adaptation*: TRAPZAL

*Adaptation number*: 0001

*Reference to original program*:

*Title of program*: KRONIG

*Catalogue number*: ACMN

*Reference in CPC*: 13 (1977) 203

*Author of original program*: S.J. Collocott

*No. of cards required to effect adaptation (including directive cards)*: 15

*Additional keywords*: trapezoidal summation

*Purpose of the adaptation*
The program KRONIG [1] shows how the Kramers–Kronig (K–K) transforms may be simply calculated using a Fourier method. The adaptation, TRAPZAL is an alternative method which uses a trapezoidal summation [2] to calculate the K–K transform. TRAPZAL has the advantage that it is numerically simpler than KRONIG and it requires fewer points to compute the K–K transform. There is very little difference in the accuracy of the two methods.

*References*

[1] S.J. Collocott, Comput. Phys. Commun. 13 (1977) 203.
[2] H.C. Bolton, G.J. Troup and G.V.H. Wilson, Phil. Mag. 9 (1964) 591.

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Computer Physics Communications 17 (1979) 397–412
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# CASTOR 2: A TWO-DIMENSIONAL LASER TARGET CODE

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*(Euratom/UKAEA Fusion Association)*

and

N.K. WINSOR
*Naval Research Laboratory, Washington, DC, USA*

Received 9 February 1979

## PROGRAM SUMMARY

*Title of program*: CASTOR 2

*Catalogue number*: ABUY

*Computer*: ICL 4/70; *Installation*: UKAEA Culham Laboratory (the program can be used on any computer equipped with the OLYMPUS system)

*Operating system*: ICL Multijob

*Programming languages used*: OLYMPUS FORTRAN

*High speed store required*: 110 000 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 13 600

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Refs. in CPC* |
|---|---|---|
| ABUF | OLYMPUS (ICL 4/70) | 7 (1974) 245 |
| ABUJ | OLYMPUS (IBM 370/165) | 9 (1975) 51 |
| ABUK | OLYMPUS (CDC 6500) | 10 (1975) 167 |
| ABUV | TRIP 1 | 16 (1978) 129 |

Alternative versions already published

*Keywords*
plasma physics, thermonuclear fusion, laser fusion, lasers, laser target, two-dimensional diffusion, implicit, ICCG, ionization, flux corrected transport, rezoning

*Nature of physical problem*
The purpose of CASTOR 2 is to calculate the behaviour of laser-irradiated targets of moderate to high atomic $Z$. A two-dimensional MHD model in cylinder $(r, z)$ geometry including three temperatures, time-dependent atomic physics, hydrodynamics and radiation transport-emission, is used in CASTOR 2. The code is meant to serve as a framework for further studies of laser targets either through manipulation of the existing physics and parameters or via extensions to both.

*Method of solution*
The target is described by 8 main variables which are functions of time $t$ and the two spatial coordinates $r$ and $z$. The solution is split into two stages. In stage I (diffusion stage) magnetic source terms to the diffusion equations are treated by the

ADI method while the diffusion of the three temperatures and the magnetic field is done by either a splitting method or the ICCG method [1]. In stage II (hydrodynamics) the hydrodynamic motion is solved by the FCT algorithms of Boris and Book [2].

*Restrictions on the complexity of the problem*
Version 2 of CASTOR which supersedes an unpublished version 1 provides a framework for laser target calculations. Because of the complexity of the physics included in the model there is no guarantee that any calculation can be completed by the code. It may therefore be necessary to "trim" calculations as explained in file INTRO of the code listing. The basic operation of the code follows the OLYMPUS pattern [3].

Double precision should be used on computers with only 32 bits per word. The code conserves energy exactly so that error I displayed by the diagnostics should remain at round-off level. This provides a useful check against errors arising from modifications to the code. The accuracy of the calculation is highly sensitive to the precision level used (i.e. no. of bits per word) and two parameters RNDOFF and DELTA control the accuracy. The accuracy also depends on the number of meshpoints used as well as the timestep control settings.

*Typical running time*
Execution times depend on the amount of physics included and on the number of meshpoints used. The execution times given below are obtained on the Culham Laboratory ICL 4/70 for the CASTOR 2 code with a mesh of 10 by 40, running in modes of increased complexity and these times are expressed in seconds per timestep. Because of the complexity of the physics these figures are only for guidance since convergence control, timestep control etc., may decrease or increase the execution time in a particular calculation.

| | | |
|---|---|---|
| 1 | 1-temperature, diffusion by splitting, no hydrodynamics | 3.5 |
| 2 | 2-temperatures, diffusion by ICCG, no hydrodynamics | 8.8 |
| 3 | 3-temperatures, diffusion by splitting, no hydrodynamics | 10.5 |
| 4 | 2-temperatures and magnetic field, diffusion by ICCG, hydrodynamics | 18.0 |
| 5 | 3-temperatures, ICCG, hydrodynamics, magnetic field, smoothing | 25.0 |

*References*

[1] D.S. Kershaw, J. Comput. Phys. 26 (1978) 43.
[2] J.P. Boris and D.L. Book, J. Comput. Phys. 11 (1973) 38.
[3] J.P. Christiansen and K.V. Roberts, Comput. Phys. Commun. 7 (1974) 244.

Computer Physics Communications 17 (1979) 413–422
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# LATTICE DYNAMICS OF ZINCBLENDE STRUCTURE COMPOUNDS
## II. SHELL MODEL

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and

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Received 13 October 1978, in revised form 11 December 1978

## PROGRAM SUMMARY

*Title of program*: LATTICE DYNAMICS – SHELL MODEL

*Catalogue number*: ACUC

| *Computer*: | *Installation*: |
|---|---|
| CDC Cyber 173 | University of Aarhus |
| IBM 370/168 | CNRS-CIRCE, Orsay |

*Operating system*: CDC: Kronos, Version 2.1.2-419-C3; IBM: OS-VS2, Release 3.7, JES 3 2.0.1

*Programming language used*: FORTRAN IV

*High speed store required*: 16 k (CDC), 89 k (IBM)

*No. of bits in a word*: 60 (CDC), 32 (IBM)

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: lineprinter

*No. of cards*: 601

*CPC Library subprograms used*:
*Cat. no.:* ACMP; *Title*: LATTICE DYNAMICS OF ZINCBLENDE; *Ref. in CPC*: 16 (1979) 181

*Keywords*: solid state, semiconductors, lattice dynamics, phonons, dispersion curves, dynamical matrix, zincblende structure, diamond structure, shell model

*Nature of physical problem*
In many kinds of calculations one needs the phonon frequencies and possibly also the phonon eigenvectors. The present program will calculate both quantities for a given wave vector $\boldsymbol{k}$, in crystals of zincblende and diamond structure.

*Method of solution*
Dynamical matrix is calculated in terms of either 14-parameter shell model [1] or Overlap Valence Shell Model [2] or 'general' shell model [3,4] (35 tensor-force parameters extending to second neighbours).

*Typical running time*
0.5 s per phonon (CDC), 0.2 s (IBM).

*Restrictions on the complexity of the problem*
Zincblende structure and diamond structure compounds. *Rigid* shell model (i.e. neither breathing degrees of freedom, nor quadrupolar deformations are allowed).

*References*

[1] G. Dolling and J.L.T. Waugh, in: Lattice dynamics, ed. R.F. Wallis (Pergamon Press, London, 1965) p. 19;
For review see also D.L. Price, J.M. Rowe and M. Nicklow Phys. Rev. B3 (1971) 1268.
[2] L.A. Feldkamp, D.K. Steinman, N. Vagelatos, J.S. King and G. Venkataraman, J. Phys. Chem. Solids 32 (1971) 1573;
K. Kunc and H. Bilz, Proc. Conf. on Neutron scattering, ed. R.M. Moon (Oak Ridge Nat. Lab., 1976) p. 195.
[3] S.K. Sinha, CRC Crit. Rev. Solid State Sci. 3 (1973) 273.
[4] A.A. Maradudin, E.W. Montroll, G.H. Weiss and I.P. Ipatova, Solid state physics, eds. H. Ehrenreich et al., Suppl. 3, 2nd ed. (Academic Press, New York, London, 1971).

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## ERRATUM NOTICE

*Title of manuscript*: II. A program for computing normal modes of molecules, crystal phonon dispersion relations and structure factors for neutron inelastic scattering.

*Author*: F.Y. Hansen

*Reference*: Comput. Phys. Commun. 14 (1978) 219

*Title of program*: FYFRE

*Catalogue number*: ACXR

## ERRATUM NOTICES

*Title of manuscript*: Multistate molecular treatment of atomic collisions in the impact parameter approximation I – Integration of coupled equations and calculation of transition amplitudes for the straight line case

*Authors*: C. Gaussorgues, R.D. Piacentini and A. Salin

*Reference*: Comput. Phys. Commun. 10 (1975) 223

*Title of program*: PAMPA

*Catalogue number*: ACWJ

*Title of manuscript*: Multistate molecular treatment of atomic collisions in the impact parameter approximation. III – Integration of coupled equations and calculation of transition amplitudes for Coulomb trajectories

*Authors*: R.D. Piacentini and A. Salin

*Reference*: Comput. Phys. Commun. 12 (1976) 199

*Title of program*: TANGO

*Catalogue number*: ACWU

*Title of manuscript*: An adaptation of ACRZ to calculate electric quadrupole oscillator strengths

*Author*: M. Godefroid

*Reference*: Comput. Phys. Commun. 15 (1978) 275

*Title of the adaptation*: Quadrupole transitions

*Adaptation number*: ACRZ0001

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# A PROGRAM GENERATOR FOR THE INCOMPLETE *LU* DECOMPOSITION-CONJUGATE GRADIENT (ILUCG) METHOD

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Received 30 March 1978; in revised form 7 February 1979

## PROGRAM SUMMARY

*Title of program*: GENLU

*Catalogue number*: ABSE

*Computer*: PDP 10; *Installation*: Computer Centre, Plasma Physics Laboratory, Princeton University, James Forrestal Campus, P.O. Box 451, Princeton, NJ 08540, USA

*Operating system*: TOPS-10, version 6.03

*Programming language used*: FORTRAN IV

*High speed storage required*: 11 280 words for source module, 14 463 words for relocatable module

*Number of bits in a word*: 36

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter

*Number of cards in combined program and test deck*: 2070

*Keywords*: general purpose, matrix, linear sparse system, incomplete LU decomposition, conjugate gradient, code generator

*Nature of physical problem*
The program generator GENLU and the resultant Incomplete *LU* Decomposition-Conjugate Gradient (ILUCG) Solver SOLLU are applicable to a wide range of physical problems, in particular those modelled by partial differential equations. Elliptic, parabolic and hyperbolic types of equations are all covered since the method can be used to solve any sparse system of linear equations with a non-singular matrix of coefficients. In practice it is desirable that the matrix be diagonally dominant because otherwise its incomplete *LU* decomposition may be a very poor approximation to the exact *LU*.

*Method of solution*
The incomplete *LU* decomposition-conjugate gradient method, the ILUCG method, of Kershaw [1] is used **. This is a generalization of the incomplete Cholesky conjugate gradient method of Meijerink and Van der Vorst [2] which applies only to positive definite symmetric matrices.

*Restrictions on the complexity of the problem*
The method will work for systems with any degree of sparsity. However, the particular generator is most efficient for sparse matrices with a definite band structure with only a few zeros in the sub-diagonals containing non-zero coefficients. If these conditions are not satisfied an unnecessarily large amount of redundant expressions will be computed. The generator GENLU also assumes a repetitive block structure, discussed in detail in the long write up. At present the dimensions of arrays which describe the beginnings and ends of diagonal bands in the problem matrix are set at 20, which means not more than 40 bands can appear in the problem matrix. This number, however, can easily be varied by re-dimensioning the common list in GENLU.

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* This work was supported by United States Department of Energy, Contract No. EY-76-C-02-3073; also Lawrence Livermore Laboratory, Livermore, CA 94550, Contract No. W-7405-ENG-48.

** Since submission to the journal the program has been modified to use an alternative ILUCG algorithm which minimizes in the Euclidean norm [3].

*References*

[1] D.S. Kershaw, J. Comput. Phys. 26 (1978) 43.

[2] J.A. Meijerink and H.A. van der Vorst, Math. Comput. 31 (1977) 148.

[3] M. Petravic and G. Kuo-Petravic, J. Comput. Phys. (1979) in press.

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# ANALYSIS OF FARADAIC IMPEDANCE EXPERIMENTAL MEASUREMENTS

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and

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Received 9 June 1978; in revised form 27 February 1979

## PROGRAM SUMMARY

*Title of program*: BATAN

*Catalogue number*: ACZA

*Computer*: IBM 1130; *Installation*: Centro de Processamento de Dados, Campus de São Carlos, São Carlos – SP

*Operating System*: IBM 1130 disc monitor system, version 2

*Program language used*: FORTRAN

*High speed storage required*: 13 kwords

*No. of bits in a word*: 16

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter, plotter IBM-1627

*No. of cards in combined program and test deck*: 1000

*Card punching code*: Hollerith

*Keywords*: electrochemistry, electrode kinetics, electrode impedance, Randles, Sluyters

*Nature of the physical problem*
This program calculates the kinetic parameters (rate constant and transfer coefficient) of a simple electrode reaction from alternating current measurements [1].

*Method of solution*
Randles' method [2] and Sluyters' method [3] are used for the calculation of the exchange current density. The method of Biegler and Laitinen [4] is then used to calculate the rate constant and the transfer coefficient of the simple electrode reaction.

*Typical running time*
On the IBM-1130 machine, one run takes about 20 min.

*References*

[1] M. Sluyters-Rehbach and J.H. Sluyters, in: Electroanalytical chemistry, vol. 4, ed. A.J. Bard (Marcel Dekker, New York, 1970).

[2] J.E.B. Randles, Discussions Faraday Soc. 1 (1947) 11.

[3] J.H. Sluyters, Rec. Trav. Chim. 79 (1960) 1092.

[4] T. Biegler and H.A. Laitinen, Anal. Chem. 37 (1965) 572.

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# A PROGRAM TO GENERATE CLOSED BASIC DIAGRAMS FOR PRODUCT OPERATORS *

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and

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Received 15 November 1978; in revised form 28 February 1979

## PROGRAM SUMMARY

*Title of program*: CONTRACTION–BASIC–DIAGRAM

*Catalogue number*: ACZI

| *Computer*: | *Installation*: |
|---|---|
| 360/65 | University of Rochester |
| 370/165 | University of Toronto |
| 3033 | Louisiana State University |

*Operating system*: HASP/OSMVT, MVS/JES2

*Programming language used*: FORTRAN IV

*High speed storage required*: 13 kwords (52 kbytes)

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, printer, disc

*No. of cards in combined program and test deck*: 726

*Keywords*: general purpose, statistical spectroscopy, scalar trace, configuration trace, perturbation theory, Hugenholtz diagram, basic diagram, matrix element symmetry, unitary symmetry, permutation

*Nature of physical problem*
Operators, referred to here as basic operators, such as Hamiltonian, electromagnetic transition and nucleon transfer, are defined in terms of products of single particle creation and annihilation operators (and their matrix elements). In many physical problems, it is necessary to evaluate the scalar and configuration traces of a product of basic operators. The easiest way to achieve this is to find all the diagrams, i.e., complete contractions among the single particle operators. Because of symmetry relations, such as permutations, matrix element and unitary symmetries, many diagrams are related and the minimum set from which all other diagrams can be generated is called the basic diagrams. Consequently, the capability to find all the basic diagrams for an arbitrary product operator is most essential in trace evaluations.

*Method of solution*
A digital representation is devised so that a definite order between different diagrams can be established. A basic diagram is recognized by the fact that the application of symmetry considerations can only produce diagrams later in the order. The algorithm for programming on the computer is made efficient by making all possible attempts, while the diagram is being generated, to recognize the pattern for a diagram to be rejected as a basic one.

*Restrictions on the complexity of the problem*
The dimensions in the program restrict the number of basic operators in a product to be no more than 20 and the total number of single particle operators to be no more than 40. These restrictions can be easily removed by changing the dimension specifications in the program. The number of single particle operators in any one basic operator is restricted to be less than or equal to 4.

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* Work supported in part by NSF of USA and NRC of Canada.

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# CHEBYSHEV EXPANSION OF THE ASSOCIATED LEGENDRE POLYNOMIAL $P_L^M(x)$ [*]

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Received 13 February 1979

## PROGRAM SUMMARY

*Title of program*: PLMCHB

*Catalogue number*: ACZN

*Computer*: IBM 370–168

*Installation*: Gesellschaft für Schwerionenforschung mbH, Darmstadt

*Operating system*: OS/VS2 RELEASE 3.7

*Programming language used*: FORTRAN

*High speed storage required*: 575 384 bytes for extended precision version

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: Card reader, line printer

*No. of cards in program*: 479

*Keywords*: associated Legendre polynomial, Chebyshev expansion, coefficients by recurrence

*Nature of problem*
Numerical evaluation of the associated Legendre polynomial $P_L^M(x)$.

*Method of solution*
Expansion of $P_L^M(x)$ in Chebyshev polynomials and evaluation of the coefficients by recurrence.

*Restrictions on the complexity of the problem*
Ranges confined to $0 \leqslant x \leqslant 1$, $0 \leqslant L \leqslant 250$ and $0 \leqslant M \leqslant 10$ with even values of $M$ only.

*Typical running time*
For the test case 1.27 s.

*Unusual features of the program*
The high speed storage requirement can be reduced by the user – the main contributing factor being array APO in COMMON CB8.

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[*] Work sponsored by the Bundesministerium für Forschung und Technologie.

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# CHEBYSHEV SERIES FOR THE SPHERICAL BESSEL FUNCTION $j_l(r)$ *

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Received 12 July 1978; in revised form 13 February 1979

## PROGRAM SUMMARY

*Title of program*: JLRCHB

*Catalogue number*: ACZM

*Computer*: IBM 370-168

*Installation*: Gesellschaft für Schwerionenforschung mbH, Darmstadt

*Operating system*: OS/VS2 RELEASE 3.7

*Programming language used*: FORTRAN

*High speed storage required*: 91700 bytes for extended precision version.

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 415

*Keywords*: General purpose, spherical Bessel function, Chebyshev series, coefficients by recurrence

*Nature of the problem*
Numerical evaluation of the spherical Bessel function $j_l(r)$.

*Method of solution*
Expansion of $j_l(r)$ in series of Chebyshev polynomials and evaluation of the coefficients by recurrence.

*Restrictions on the complexity of the problem*
Ranges confined to: $0 \leqslant l \leqslant 20$ and $0 \leqslant r \leqslant 72$ but readily extendable, subject only to the restrictions of available machine precision and exponentiation range.

*Typical running time*
Dependent on required range and accuracy: for the test case with extended precision and accuracy of thirty figures it is 2.02 s of which 1.14 s is for calculation of the expansion coefficients.

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* Work sponsored by the Bundesministerium für Forschung und Technologie.

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# FROZEN CORE HARTREE–FOCK PROGRAM FOR ATOMIC DISCRETE AND CONTINUOUS STATES *

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Received 22 November 1978; in revised form 19 March 1979

## PROGRAM SUMMARY

*Title of program*: ATOMIC FROZEN CORE HARTREE–FOCK

*Catalogue number*: AAKZ

*Computer*: CDC 3600; *Installation*: Boris Kidrich Institute of Nuclear Sciences

*Operating system*: Tape SCOPE 6.3

*Programming language used*: ALGOL 60

*High speed storage required*: 32 k

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: one or none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 571

*CPC library subprogram used (for data):*
*Cat. No.:* AAKQ; *Title*: ATOMIC SCF HARTREE–FOCK;
*Ref. in CPC*: 11 (1976) 57

*Keywords*: atomic physics, self-consistent field, Hartree–Fock (method), independent-particle approximation, single-particle model, electronic structure, atomic models, wave functions, off-diagonal energy parameters, frozen core (approximation), ground state, excited state, single-electron state, discrete state, continuous state, single-configuration approximation, atomic shell, *nl*-(sub)shell, iteration (iterative process), (many-)electron correlations, electron configuration

*Nature of physical problem*
The present program calculates the excited state Hartree–Fock (HF) radial wave function of a single-electron in the "frozen core" (FC) field of other electrons. The radial one-electron wave functions of the "frozen core" are a solution of the corresponding self-consistent field HF problem [1]. The energy eigenvalue for single-electron discrete (bound) states, or the phase shift for continuous states are also calculated.

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* Supported in part by Serbian Research Funds, Yugoslavia.

*Method of solution*

Being a linear integro–differential equation the FC HF equation is solved by iteratively solving the corresponding inhomogeneous differential equation. The differential equation is solved in the same way as in the self-consistent field HF program [1].

The off-diagonal energy parameters are also determined iteratively, while the phase shift for the continuous state is obtained by integrating the differential equation outwards, beyond the cut-off radius, until the asymptotic behaviour is reached.

*Restriction on the complexity of the problem*

It may happen that the present program does not give a solution for certain states for which it is known that some resulting off-diagonal energy parameters are approximately equal to or greater, in absolute value, than the single-particle energy (i.e., the diagonal energy parameter), as for example, for single-particle state $ns$ in the configuration $1s^2 2sns(^1S)$. The procedure for evaluation of the off-diagonal parameters does not then converge.

*Typical running time*

The total running time including compilation on the CDC 3600 computer with all peripherals connected on-line, for the excited state configurations of the nitrogen atom with 700 integration points is:

(i) about 25 min for 18 different $\nu$d radial functions of the configuration $1s^2 2s^2 2p^2 \nu d(^4P)$ (no evaluations of off-diagonal energy parameters);

(ii) about 60 min for 18 different $\nu$s radial functions of the configuration $1s^2 2s^2 2p^2 \nu s(^4P)$.

*Unusual features of the program*

The present program is so designed that the direct results of the self-consistent field HF program [1], stored on a magnetic tape, are taken for the FC states. The independent variable in both programs is $x = \alpha r + \beta \ln r$ [1], which has behaviour suitable for both small and large values of the radii $r$.

*Reference*

[1] L.V. Chernysheva, N.A. Cherepkov and V. Radojević, Comput. Phys. Commun. 11 (1976) 57.

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# LATTICE DYNAMICS OF GROUP IV SEMICONDUCTORS USING AN ADIABATIC BOND CHARGE MODEL

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Received 16 January 1979; in revised form 12 March 1979

## PROGRAM SUMMARY

*Title of program*: ADIABATIC BOND CHARGE MODEL

*Catalogue number*: ACUD

*Computer*: CDC Cyber 173; *Installation*: University of Aarhus

*Operating system*: KRONOS ver.2.1.2-419-C3

*Program language used*: FORTRAN IV

*High speed store required*: 12 k

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards*: 1437

*Keywords*: solid state, semiconductors, lattice dynamics, phonons, dispersion curves, dynamical matrix, diamond structure, adiabatic bond charge model

*Nature of physical problem*
Determination of phonon frequencies and phonon eigenvectors for semiconductors of diamond structure.

*Method of solution*
The dynamical matrix is calculated from the adiabatic bond charge model [1]. Its eigenvalues and eigenvectors are computed.

*Typical running time*
3.0 s per phonon.

*Restrictions on the complexity*
Diamond structure only.

*References*
[1] W. Weber, Phys. Rev. B15 (1977) 4789.

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# *Z*-EXPANSION OF MATRIX ELEMENTS OF ONE-ELECTRON OPERATORS FOR MANY-ELECTRON ATOMS

M.N. LEWIS
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Received 12 July 1978; in revised form 13 March 1979

## PROGRAM SUMMARY

*Title of program*: SSTR-TRANSITION GENERALIZED SUMS

*Catalogue number*: AACH

*Computer*: CDC 6400; *Installation*: Smithsonian Astrophysical Observatory, Cambridge, MA 02138, USA

*Operating system*: SCOPE

*Program language used*: FORTRAN

*High speed store required*: 50200 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: one, temporary tape

*Other peripherals used*: card reader, line printer, card punch

*No. of cards in combined program and test deck*: 2988

*Keywords*: atomic theory, *Z*-expansion, perturbation theory, one-electron operators, single particle substitutions sums, hydrogenic, continuum singularity integration

*Nature of physical problem*
Program SSTR (Substitution Sums for Transitions), computes the generalized single-particle substitution sums used in obtaining the coefficient of the second term in the *Z*-expansion of the matrix elements of one-electron operators in many-electron atoms [1]. The calculations correspond in complexity to those needed for the contributions $E_2'$ in the second-order energy, but not to those needed for $E_2''$ [1].

The program is generalized to use one-electron operators corresponding to $r^{kk}$, for brevity referred to as a "transition", from a state with quantum numbers $n_1 l_1$ to state $n_2 l_2$ in the presence of the $n_0 l_0$ core electron.

*Method of solution*
Each generalized single-substitution sum is a sum of terms of the form $R^k(\alpha, \beta, \gamma, nl)\, T^{kk}(\delta, nl)/E(\alpha + \beta - \gamma - nl)$, with $\delta = \alpha$ or $\beta$ or $\gamma$. The substituted wave functions $P(nl)$ are members of a complete set of hydrogenic wave functions and the generalized sums are found, as in program SPSS [2], by the summation over discrete $n$ from $n = l + 1$ to $n = n_{\text{ext}} - 1$, by extrapolation from $n = n_{\text{ext}}$ to $\infty$, and by integration over the continuum energy.

*Restrictions on the complexity of the problem*
For high principal quantum numbers of the fixed wave functions it may be necessary to use double precision for parts of the calculations (see section 6). For restrictions on the scaling factor SX in subroutine PRTX see section 7.

*Typical running time*
Transitions 3p-3s and 3d-3p with a 1s core electron take a total time of 3.7 s for 7 to 10 significant figures, or 2.3 s for 4 to 7 figures.

*Unusual features of the program*
Program SSTR selects the generalized sums needed for the 'transition' and can punch results on cards. SSTR could be adapted to obtain perturbation theory summations for problems with other definite hydrogenic integrals in the numerator of the expression to be summed.

*References*

[1] D. Layzer, Z. Horák, M.N. Lewis and D. Thompson, Ann. Phys. (NY) 29 (1964) 101.
[2] M.N. Lewis, Comput. Phys. Commun. 1 (1970) 265.

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# TRANSPORT PROPERTIES OF DILUTE GAS MIXTURES

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Received 27 November 1978; in revised form 3 April 1979

## PROGRAM SUMMARY

*Title of program*: GAS MIXTURE TRANSPORT PROPERTIES

*Catalogue number*: ACZO

*Computer*: ICL 1906A; *Installation*: University of Leeds

*Operating system*: George 4

*Programming language used*: FORTRAN

*High speed store required*: 43 kwords

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in a combined program and test deck*: 1148

*Keywords*: molecular physics, fluid dynamics, gas, mixture, transport properties, thermal conductivity, diffusion, thermal diffusion, viscosity

*Nature of Physical Problem*
The transport properties of a gas mixture are the thermal conductivity, viscosity and the diffusion and thermal diffusion coefficients. The program calculates these transport properties.

*Method of solution*
The transport properties may be expressed in terms of coefficients in the Sonine polynomial expansions of the unknown coefficients occurring in the solution of the perturbed form of the Boltzmann equation. The program solves matrix equations for the coefficients and hence calculates the transport properties.

*Restrictions on the complexity of the problem*
Up to ten gases may be included in the mixture. The effect of inelastic collisions of molecules is not included and elastic collisions are described by the Lennard–Jones (12–6) potential.

*Typical running time*
Forty seconds for compilation and five seconds for execution on the Leeds 1906A.

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# BESSEL FUNCTIONS $J_\nu(x)$ AND $Y_\nu(x)$ OF REAL ORDER AND REAL ARGUMENT

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Received 14 July 1978; in revised form 23 April 1979

## PROGRAM SUMMARY

*Title of program*: BESSJY

*Catalogue number*: ACZP

*Computer*: IBM 3032; *Installation*: National Research Council, Ottawa

*Operating system*: TSS/370

*Programming language used*: FORTRAN IV

*High speed storage required*: 12305 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1499

*Keywords*: general purpose, Bessel, axisymmetric, asymptotic expansion, backward recurrence, continued fraction

*Nature of physical problem*
The BESSJY package calculates Bessel functions $J_\nu(x)$ and $Y_\nu(x)$ of real order and real argument. These functions are used for the solution of potential problems in cylindrical coordinates [1].

*Method of solution*
For extremely small argument, $J_\nu(x)$ and $Y_\nu(x)$ are determined from their limiting forms for small arguments.

For small or moderately large argument, $J_\nu(x)$ is calculated by Miller's backward recurrence algorithm described by Gautschi [2], $Y_\nu(x)$ and $Y_{\nu+1}(x)$ for $|\nu| \leqslant \frac{1}{2}$ are determined from Neumann series of functions $J_{\nu+2m}(x)$ as described by Goldstein and Thaler [3], and $Y_{\nu+k}(x)$ for $k \geqslant 2$ is determined from the forward recurrence formulae.

For large argument, the Bessel functions are determined from the asymptotic expansions for large argument and the recurrence relations.

*Restrictions on the complexity of the problem*
The functions are determined only for non-negative order. $J_\nu(x)$ is determined only for non-negative argument and $Y_\nu(x)$ is determined only for positive argument. The subroutines are inefficient when both order and argument are very large.

*Typical running time*
For argument and order not both very large, the determination of a single function requires less than 1 ms. The determination of a sequence of functions requires, in addition, approximately 10 μs for each member of the sequence. Some typical CPU times are given in section 5 of the Long write-up.

*Accuracy*
The subroutines are written in double precision. For small or moderately large arguments, the accuracy obtained is approximately 14 digits.

*References*
[1] W.R. Smythe, Static and dynamic electricity (McGraw-Hill, 1968) 179.
[2] W. Gautschi, SIAM Rev. 9 (1967) 24.
[3] M. Goldstein and R.M. Thaler, Math. Tables Aids Comput. 13 (1959) 102.

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# SLIT HEIGHT SMEARING CORRECTION IN SMALL ANGLE X-RAY SCATTERING III: INTENSITY CORRECTION PROGRAM ADAPTATION TO ARBITRARY SLIT TRANSMISSION FUNCTION *

Moshe DEUTSCH
*Department of Physics, Bar-Ilan University, Ramat-Gan, Israel*

Received 22 January 1979

## ADAPTATION SUMMARY

*Title of adaptation*: CORECTSP

*Adaptation number*: 0001

*Reference to original program*:
*Catalogue number*: AASB; *Title*: CORECTEX; *Ref. in CPC*: 17 (1979) 337.

*Author of original program*: Moshe Deutsch

*Computer*: IBM 370/168; *Installation*: Bar-Ilan University Computer Center, Ramat-Gan, Israel

*High speed storage required*: 45 500 words

*No. of bits in a word*: 32

*Other peripherals used*: card reader, line printer, magnetic disk storage

*No. of cards required to effect adaptation*: 114

*CPC Library subprograms used (for data)*:
*Cat. No.*: AASD; *Title*: GTSPLINE; *Ref. in CPC*: 18 (1979) 804.

*Nature of physical problem*
Two previous papers in this series [1,2] described an implementation of the author's exact solution of the slit height smearing correction problem encountered in small angle X-ray and neutron scattering experiments [3,4]. That implementation presumed, however, that an analytic form could be found among those listed in refs. [5,6], which closely fitted the actual slit transmission function used in the experiment.

The adapted program can be used with *any* slit function and is especially useful in cases where no suitable analytic form for the slit function is available. The program yields highly accurate results, as discussed in ref. [4] and running time is less than half that of the original program.

*Method of solution*
The method is fully described in ref. [1]. The only difference is that the measured values of the slit transmission function are now fitted by a piecewise continuous cubic spline function, rather than by an analytic function. The fitting and parameter calculations are done by a separate program [7] which must be run prior to using this program. The input section of the original program and the subroutine calculating the correction function derivative were altered to accommodate the new correction function.

*Restrictions on the complexity of the problem*
As in the original program, only 250 intensity values can be corrected in a single run.

*References*

[1] M. Deutsch, Comput. Phys. Commun. 17 (1979) 337.
[2] M. Deutsch, Comput. Phys. Commun. 17 (1979) 345.
[3] M. Deutsch and M. Luban, J. Appl. Cryst. 11 (1978) 87.
[4] M. Deutsch and M. Luban, J. Appl. Cryst. 11 (1978) 98.

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* This work was supported by a grant from the United States–Israel Binational Science Foundation (BSF), Jerusalem, Israel.

[5] M. Deutsch and M. Luban, International Union of Crystallography, Supplementary Publication No. SUP 32945 (1978); copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

[6] M. Luban and M. Deutsch, (1979), to be published.

[7] M. Deutsch, Comput. Phys. Commun. 18 (1979) 149.

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# SLIT HEIGHT SMEARING CORRECTION IN SMALL ANGLE X-RAY SCATTERING IV: COMPUTATION OF THE CORRECTION FUNCTION FOR AN ARBITRARY SLIT TRANSMISSION FUNCTION *

Moshe DEUTSCH
*Department of Physics, Bar-Ilan University, Ramat-Gan, Israel*

Received 22 January 1979

## PROGRAM SUMMARY

*Title of program*: GTSPLINE

*Catalogue number*: AASD

*Computer*: IBM 370/168; *Installation*: Bar-Ilan University Computer Center, Ramat-Gan, Israel

*Operating system*: OS/VS2

*Programming language used*: FORTRAN IV G

*High speed storage required*: 27 500 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, magnetic disk storage

*No. of cards in combined program and test deck*: 1496

*Keywords*: crystallography, X-ray, scattering, diffraction, smearing, slit, small-angle

*Nature of physical problem*
The author's previously published program for correcting slit height smeared data measured in small angle X-ray scattering experiments [1] requires the use of a correction function $g(t)$, which is related to the slit transmission function $f(t)$. The present program calculates the required correction function for an *arbitrary* slit function, given its numerical values.

*Method of solution*
A piecewise cubic spline function [2] is fitted to the measured values of the slit transmission function. The fit parameters define an analytically calculated transform of the slit function, $\hat{F}$, similar to the usual Laplace transform. $\hat{F}$ is then Laplace-inverted numerically to give a set of discrete values of the correction function $g(t_i)$, $i = 1, ..., n$. Finally, another spline function is fitted to these values, yielding a continuous representation of the desired correction function $g(t)$.

*Restrictions on the complexity of the problem*
Only 100 measured values of the slit transmission function are allowed in the present version.

*Typical running time*
About 160 s for 75 transmission function values.

*References*

[1] M. Deutsch, Comput. Phys. Commun. 18 (1979) 143.
[2] M.J.D. Powell, Report No. HL67/5309 (TP307) (1967) AERE, Harwell, Didcot, Oxon OX11 0RA, England.

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* This work was supported by a grant from the United States–Israel Binational Science Foundation (BSF), Jerusalem, Israel.

Computer Physics Communications 18 (1979) 155–162
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# PROGRAM ADAPTATION: TO CALCULATE INCLUSIVE BACKWARD PROTON CROSS SECTIONS

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and

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Received 4 December 1978

## ADAPTATION SUMMARY

*Title of adaptation*: BACKWARD INCLUSIVE PROTONS

*Adaptation number*: 0001

*Reference to original program*:
*Cat. No.*: AAUR; *Title*: ONCPLT; *Ref. in CPC*: 12 (1976) 277

*Authors of original program*: K.J.M. Moriarty and J.H. Tabor

*Computer*: CDC 6600; *Installation*: University of London Computer Centre

*Number of bits in a word*: 60

*Number of cards required to effect adaptation*: 401

*CPC Library subprograms used*:

| *Cat. No.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAUN | APLOT | 9 (1975) 85 |
| AAUN0001 | POLAR PLOT AND IMPROVEMENTS | 15 (1978) 437 |

*Additional keywords*: backward single-particle-inclusive cross section, degenerate hypergeometric functions

*Nature of physical problem*
This adaptation involves the phenomenological analysis and display (via printer and graph plotter) of high-energy backward inclusive single-particle production cross sections.

*Method of solution*
The program can be run under either the fixed $t$ or the fixed $M^2$ modes for calculating differential cross sections. In the fixed $t$ mode the $t$-bin is integrated over by 8-point Gaussian quadrature. The results are plotted by using the graph plotting package APLOT and POLAR PLOT AND IMPROVEMENTS [1]. The program is compatible with the MINUIT minimization system [2].

*Restrictions on the complexity of the program*
The number of inclusive cross section data points cannot exceed 500.

*Typical running time*
The test run took 42.8 s (of which 23.8 s was compilation time).

*References*

[1] J. Anderson, K.J.M. Moriarty and R.C. Beckwith, Comput. Phys. Commun. 9 (1975) 85;
J. Anderson, R.C. Beckwith, K.J.M. Moriarty and J.H. Tabor, Comput. Phys. Commun. 15 (1978) 437.
[2] F. James and M. Roos, Comput. Phys. Commun. 10 (1975) 343.

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# EXACT FINITE RANGE DWBA FORM FACTOR FOR HEAVY-ION INDUCED NUCLEAR REACTIONS

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and

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Received 17 March 1979

## ADAPTATION SUMMARY

*Title of adaptation*: SATURN-2-FOR-EFR-DWBA

*Adaptation number*: 0001

*Reference to original program*:
*Cat. No.*: ABPA; *Title*: SATURN-1-FOR-EFR-DWBA;
*Ref. in CPC*: 8 (1974) 349

*Authors of original program*: T. Tamura and K.S. Low

*High speed store required*: 39 872 words

*Other peripherals used*: card reader, line printer

*Number of cards required to effect adaptation (including directive cards)*: 869

*Method of solution*
Calculation of the form factor involves a four-fold integral, though it can normally be reduced to a sum of single-fold integrals. When the original program is used for cases with large angular momentum transfer the sum results in a severe cancellation between summands, making the results inaccurate. The present program uses a new coordinate system in performing the above integral and makes it possible to avoid the difficulty.

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* Supported in part by the U.S. Department of Energy.

Computer Physics Communications 18 (1979) 215–244
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# A GUIDE TO ANALYTIC EXTRAPOLATIONS

## Part I: A program for optimal extrapolation to interior points

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*Th. Div., CERN, Geneva, Switzerland*

Received 27 January 1978; in revised form 8 June 1979

## PROGRAM SUMMARY

*Title of program*: ANALYT

*Catalogue number*: AAUT

*Computer*: IBM 370/3033, Kernforschungszentrum, Karlsruhe, tested also on UNIVAC 1108 and on CDC 6600 and CDC 7600

*Operating system*: OS/VS 2, Compiler Fortran H opt. (2)

*Programming language used*: FORTRAN IV

*High speed storage required* (in GO step): 212 k *

*No. of bits in k-word*: 8 bits in a byte, 1024 bytes in 1 k

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test decks*: 2500

(*No. of cards of the* ANALYT *deck*: 1800)

*Key-words*: nuclear physics, scattering amplitude, analytic continuation, inverse problems, stability, dispersion relations, functional methods, zeros, poles

*Nature of the physical problem*
In the scattering theory of elementary particles as well as in any other branch of physics in which the analyticity of some function of physical interest has been established, one is often faced with the practical question of continuing data given on parts of the cuts, in an analytic way towards some interior points of the analyticity domain. Since this problem is "ill posed" in the Hadamard sense, in order to get sensible predictions, one has to "stabilize" the output by means, for instance, of a boundedness condition, given on those parts of the cuts where the actual data is lacking (e.g. a Froissart bound).

The present program processes the input data and the stabilizing condition in an optimal function-analytic way, yielding estimates of analytic continuations in any desired interior point, as well as the value of some important nonlinear functionals [1] which "measure" the "analyticity" of the input. These numbers might then be used to correlate in an analytic way data spread on different energy regions, to get informations about the asymptotics, or to find zeros and poles of the scattering amplitude.

*Method of solution*
Calling once the subroutine ANALYT, all the pertinent information (the complex-valued data and the points where it is given, the form of the error corridor and the function-bounds), is loaded. Then, according to the name of the extrapolation function one calls, one gets either the PoissoN weighted EXtrapolation [2], PNEX($s$), which optimizes dispersion relations versus the uniform ($L^{\infty}$) norm, the CauchY weighted EXtrapolation, CYEX($s$), (optimization versus the $L^2$ norm, of Cutkosky's modified $\chi^2$-test, see ref. [3]), or the Central Analytic EXtrapolation, CAEX($s$), which gives at any point $s$, the center of gravity of the (complex) values taken there *by all* the analytic functions compatible with the initial data

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* The memory requirements may be considerably lowered if the dimension statements are changed accordingly (see outlook of ref. [1]).

and boundedness condition [4]. The values of the other four external functions described in part 1, may be computed by calling the corresponding entry points. Further, calling EMZERO/or EPZERO/ (see part 2 [1]), one computes a number (≡ the width of the smallest bound, or smallest error corridor, still compatible with the initial data and with the analyticity), which might be used then to recognize "good" (i.e. "analytical") data from "wrong" ones. A further facility permits to see whether the data *and* the analyticity condition is compatible or not with the existence of a (or a pair of) zero(s) or pole(s), placed at some given point $s_{\mathrm{zero}}$.

*Restrictions on the complexity of the problem*
None, provided sufficient data points and suitable dimensions were taken (in the test run these numbers were 181 and 501, respectively).

*Typical running times*
The Cauchy weighted or the Poisson weighted extrapolations need only some 0.2 s per point, but the central analytic or the other special extrapolations are more time consuming (approx 1 min, see remark 3.1.0). Their subsequent calls need again only 0.2 s per extrapolated point. Some 10 s are necessary for EMZERO/EPZERO. Further details might be found in the two test programs descriptions at the end of ref. [1].

*References*

[1] I. Caprini, M. Ciulli, S. Ciulli, C. Pomponiu, M. Sararu and I.S. Stefanescu, Comput. Phys. Commun. 18 (1979).
[2] S. Ciulli and J. Fischer, Nucl. Phys. B24 (1970) 537.
[3] R.E. Cutkosky, Ann. Phys. 54 (1969) 110.
[4] S. Ciulli and G. Nenciu, J. Math. Phys. 14 (1973) 1675; S. Ciulli, C. Pomponiu and I.S. Stefanescu, Phys. Rept. 17C (1975) 133.

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# MCBP – A PROGRAM TO CALCULATE ANGULAR COEFFICIENTS OF THE BREIT INTERACTION BETWEEN ELECTRONS IN THE LOW ENERGY LIMIT

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and

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Received 9 March 1979

## PROGRAM SUMMARY

*Title of program*: MCBP–BREIT ANGULAR COEFFICIENTS

*Catalogue number*: AAAL

*Computer*: IBM 360/195; *Installation*: Rutherford Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, UK

*Operating system*: OS/360, HASP

*Programming language used*: FORTRAN IV

*High speed storage required*: 176 kbytes (execution only)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes used*: none

*Other peripherals used*: card reader, line printer, disc file (if available)

*No. of cards in combined program and test deck*: 1974

*CPC Library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAHD | NJSYM | 8 (1974) 151 |
| ACRI | CFPJJ–CFP IN JJ-COUPLING | 4 (1972) 377<br>14 (1978) 311 |
| ACWE | MCP75 | 11 (1976) 397<br>14 (1978) 312 |

*Keywords*: atomic, configuration interaction, Racah, fractional parentage, recoupling coefficients, Slater integrals, complex atoms, relativistic, Dirac equation, wave function, retarded interaction, Breit, *jj*-coupling, theoretical methods

*Nature of physical problem*
The retarded interaction between a pair of electrons makes a non-negligible contribution to atomic energy levels especially in processes such as X-ray emission and absorption and Auger spectroscopy, involving inner shell holes. This program handles the algebraic part of this calculation using the formulation of Grant and Pyper [1] and lists the coefficients of radial integrals in a form suitable for use with the wavefunctions produced by multiconfiguration Dirac–Fock programs, such as that of Grant, Mayers and Pyper [2]. The input to this program is identical with that used in MCP75 [3,4].

*Restrictions on the complexity of the problem*
The program assumes that all open shell configuration state functions are formed from the same orthonormal set of basis orbitals. The number of electrons in a shell having $j \geqslant \frac{9}{2}$ is restricted to be not greater than 2 by the available c.f.p. tables. The present version allows up to 10 open or closed shell orbitals and 30 configurational states with up to 6000 coefficients. These numbers can be changed by the user. It is advisable to ensure that the library subprograms AAHD and ACRI have been converted to use double precision floating point arithmetic when implementing the package on IBM machines.

*References*

[1] I.P. Grant and N.C. Pyper, J. Phys. B9 (1976) 761.
[2] I.P. Grant, D.F. Mayers and N.C. Pyper, J. Phys. B9 (1976) 2777.
[3] I.P. Grant, Comput. Phys. Commun. 5 (1973) 263.
[4] I.P. Grant, Comput. Phys. Commun. 11 (1976) 397.

Computer Physics Communications 18 (1979) 261–275
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# PLOT PROGRAM FOR LAUE PATTERNS AND STEREOGRAPHIC PROJECTIONS

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Received 23 February 1979

## PROGRAM SUMMARY

*Title of program*: PLOMAC

*Catalogue number*: AAQE

*Computer*: IBM 370-168; *Installation*: Zentral-Institut für Angewandte Mathematik, Kernforschungsanlage Jülich

*Operating system*: MVS

*Program language used*: FORTRAN IV

*High-speed storage required*: 332 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: 1 (for the CALCOMP plotter)

*Other peripherals used*: card reader, line printer, CALCOMP 1670/900 microfilm plotter

*No. of cards in combined program and test deck*: 3099

*Keywords*: solid state physics, crystallography, crystal structures, crystal diffraction, X-ray diffraction, orientation of single crystals, single crystal surface preparation, gnomonic and stereographic projections, flat and cylindrical Laue photographs, transmission and back-reflection Laue techniques.

*Nature of physical problem*

The program simulates Laue patterns of any crystal type and of any crystal orientation. With the aid of a catalogue of plotted Laue diagrams the orientation of single crystals can be carried out quite easily by the direct comparison of the Laue photographs with the diagrams. This can be performed even by people with no previous experience in this field.

*Method of solution*

Trigonometric functions, vector algebra and formulas of analytic geometry are used. Transformation equations, relating the Miller indices of any crystal type with those in a rectangular Cartesian coordinate system, are introduced. The coordinates for the Laue spots are evaluated by the program. They are not read from cards or from a magnetic tape [1]. The complete symmetry rather than the exact intensity of the plotted spots is essential for the crystal orientation method.

*Typical running time*

≈ 30 s for one diagram.

*Restrictions on the complexity of the problem*

The structure factor and the crystal parameters of the unit cell must be known. There are ten structure factors for the most common crystal types in the program which can be called up ad-lib. These can be replaced by 17 structure factors for less common crystal types on comment cards or by others, if needed.

*Unusual features of the program*

The software subprograms for the CALCOMP plots (California Computer Products, In.) CALCMP, NUMBR, SYMBL, FAKT, CALIN, FRAMAD, CALEND [1] must be replaced if other plotters are used.

*References*

[1] M. Canut-Amoros, Comput. Phys. Commun. 1 (1970) 293.

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# CALCULATION OF CRYSTAL ORIENTATIONS USING LAUE PATTERNS

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Received 23 February 1979

## PROGRAM SUMMARY

*Title of program*: COL

*Catalogue number*: AAQF

*Computer*: IBM 370-168; *Installation*: Zentral-Institut für Angewandte Mathematik, Kernforschungsanlage Jülich

*Operating system*: MVS

*Program language used*: FORTRAN IV

*High-speed storage required*: 200 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 358

*CPC library subprogram used (for data)*: *Cat. no.*: AAQE; *Title*: PLOMAC; *Ref. in CPC*: 18 (1979) 812

*Keywords:* solid state physics, crystallography, crystal structures, crystal diffraction, X-ray diffraction, orientation of single crystals, single crystal surface preparation, flat and cylindrical Laue photographs, transmission and back-reflection Laue technique

*Nature of physical problem*
The program evaluates the orientation of single crystals numerically.

*Method of solution*
This method uses cylindrical, flat transmission or flat back-reflection Laue photographs. The Miller indices and the coordinates of three Laue spots on the film must be known. The indexing of the Laue spots can be performed by using the plot program of the author described in this issue of CPC. The crystal parameters of the unit cell have to be inserted into the program. In the calculations, trigonometric functions, vector algebra, formulas of analytic geometry and transformation equations relating the Miller indices of any crystal type with those of a rectangular Cartesian coordinate system are used. The transformations are performed in both directions. The crystal orientation in components of a vector given in the coordinate system of the crystal axes will be printed out in fixed point numbers. In order to obtain the Miller indices of the required orientation, those numbers can be converted into integers by a common factor. Since the precision wanted for this statement may be varying, this must be performed by the user of the program.

*Typical running time*
Less than 1 s.

*Restrictions on the complexity of the problem*
The crystal parameters of the unit cell must be known. The three indexed Laue spots on the photograph are not allowed to be reflections from equivalent lattice planes.

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# DOMUS – A PROGRAM FOR THE ANALYSIS OF TWO-DIMENSIONAL SPECTRA

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*Joint Institute for Nuclear Research, Laboratory of Computing Technique and Automation, Dubna, USSR*

Received 16 February 1979; in revised form 14 June 1979

## PROGRAM SUMMARY

*Title of program*: DOMUS

*Catalogue number*: ABAB

*Computer*: CDC-6500; *Installation*: JINR, Laboratory of Computing technique and automation, Dubna

*Operating system*: SCOPE

*Programming language used*: FORTRAN 4

*High speed storage required*: 32 kwords

*No. of bits in a word*: 60

*Overlay structure*: none

*No of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 2596

*Keywords*: nuclear, molecular, spectrum, emission, absorption, data analysis, spectrometry, multidimensional data, spectrum analysis, mixture decomposition

*Nature of physical problem*
The program decomposes two-dimensional spectra into the components of interest and that of background, and evaluates such quantities as volumes, two-dimensional positions and widths of the components of interest.

*Method of solution*
The program inputs the models of the components of interest, which may be constructed using either analytical functions, describing the component shape, or experimentally measured histograms, representing that shape, and fits the spectrum (divided into parts), estimating the characteristics of the relations between the models and the real images in such a way that these estimates determine at the same time the values of quantities of interest: peak volume, position and width.

*Restrictions on the complexity of the problem*
The maximum number of components in the analyzed spectrum interval = 12.

*Typical running time*
The average time is about 10 s per component.

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Computer Physics Communications 18 (1979) 287–296
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# ECSIMPACT, A SPECIAL VERSION OF PROGRAM IMPACT FOR CDC MACHINES WITH EX-CORE MEMORY

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Received 28 March 1979

## PROGRAM SUMMARY

*Title of program*: ECSIMPACT

*Catalogue number*: ACZK

*Computer*: CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: SCOPE 2.1.4

*Programming language used*: FORTRAN IV

*High speed storage required*: 20 kwords (decimal)

*Number of bits in a word*: 60

*Overlay structure*: overlaid

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, 6 auxiliary (disk) files

*Number of cards in combined program and test deck*: 6682

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACYF | IMPPRO | 15 (1978) 23 |
| ACYF0001 | ADAPT IMPPRO FOR ECSIMPACT | this paper |

*Reference to other published version of this program*:
*Cat. no.*: ACYE; *Title*: IMPACT; *Ref. in CPC*: 15 (1978) 23

*Keywords*: atomic, structure, electron–atom, electron–ion, scattering

*Nature of the physical problem*
Solution of coupled second order integro–differential equations used to obtain wave functions for a system of e + atom or ion. Full description in ref. [1].

*References*

[1] M.A. Crees, M.J. Seaton and P.M.H. Wilson, Comput. Phys. Commun. 15 (1978) 23.

## ADAPTATION SUMMARY

*Title of adaptation*: ADAPT IMPPRO FOR ECSIMPACT

*Adaptation number*: 0001

*Reference to original program*: *Cat. no.*: ACYF; *Title*: IMPPRO; *Ref. in CPC*: 15 (1978) 23

*Authors of original program*: M.A. Crees, M.J. Seaton and P.M.H. Wilson

*Number of cards required to effect the adaptation (including the derivative cards)*: 39

*Purpose of the adaptation*

To make the processor insert the special array sizes required by ECSIMPACT, which is a version of the program IMPACT. ECSIMPACT is published in this issue of CPC. The adapted processor will still work for program IMPACT as well. The switch for ECSIMPACT is effected by punching a 1 into column 50 of the second data card to the adapted IMPPRO. The test run output is included with that of ECSIMPACT.

*Unusual features of the adaptation*

The command cards to effect the adaptation are standard CDC UPDATE commands.

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# RADIATION POTENTIAL OF A POINT ANTENNA IMMERSED IN DRIFTING COLD OR HOT (HYDRODYNAMICAL) PLASMA

E. FIJALKOW * and G. MOURGUES **
*Laboratory CRPE/CNRS, 45045 Orleans Cedex, France*

Received 23 May 1979

## PROGRAM SUMMARY

*Title of program*: DRFT

*Catalogue number*: ABUZ

*Computer*: IBM 370/168 × 2, CII-HB 10070, double precision; *Installation*: CIRCE Campus du CNRS ORSAY, Université d'Orléans

*Operating system*: MVS-JES3

*Programming language used*: FORTRAN IV (H level)

*High speed storage required*: 59 kbytes

*No. of bits in a word*: 64

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 536

*Keywords*: plasma physics, drift velocity, forced potential, point antenna

*Nature of physical problem*
Computation at arbitrary given distances from the source of the radiation diagrams of the potential forced by a pulsating point antenna immersed in a hot uniformly drifting plasma.

*Method of solution*
The choice of a Water Bag (W.B.) model to describe the distribution function allows us to calculate the dispersion relation $D(\boldsymbol{k}, \omega)$ in "$\boldsymbol{k}$" space, and the value of the potential $V(\boldsymbol{k}, \omega)$ follows immediately [1]. The potential in ordinary space, $V(x, \omega)$ is obtained by an inverse Fourier transform on $\boldsymbol{k}$. The integrals are performed in a cylindrical coordinate system: $K_\perp$, $\theta'$, $K_\parallel$. $K_\parallel$ is taken in the direction of the drift. The integration over the $\theta'$ variable is performed anlytically and results in the Bessel function of zero order. The second integration in $K_\parallel$ for fixed values of $K_\perp$ is done by the method of residues and a table for different values of $K_\perp$ is constructed. The last integral (in $K_\perp$ variable) is calculated numerically, by Romberg's method for small values of $K_\perp X_\perp$, and by Filon's method for large values. Non-tabulated intermediate points are given by a third order Spline interpolation method.

A thermal parameter, $\rho$, defined as the thermal velocity divided by the drift velocity may take arbitrary values (the cold plasma case is the limiting value $\rho = 0$).

*Restriction on the complexity of the problem*
The only restrictions on the program are:
1) $\omega$ must be greater than the plasma frequency $\omega_p$
2) $\theta$ must be different from $\pi/2$.

*Typical running time*
The test run output (full radiation diagram $\theta$ varying from zero to 180°, one distance from the source) about 62.87 s.

*Reference*
[1] G. Mourgues, E. Fijalkow and M.R. Feix, Plasma Phys. (1979) submitted.

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* Université d'Orléans, UER Sciences.
** Université de Clermont-Ferrand, IUT de Montluçon.

Computer Physics Communications 18 (1979) 353–362
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# NUMERICAL MODELLING OF A CHEMICAL PLASMA

## I. REACS: A program to generate all reactions which take place in a plasma of given chemical content

S.A. ROBERTS

*Department of Computer Studies, The University, Leeds, UK*

Received 9 October 1978; in revised form 9 February 1979

## PROGRAM SUMMARY

*Title of program*: REACS

*Catalogue number*: ACZD

*Computer*: ICL 1906A; *Installation*: University of Leeds Computing Centre

*Operating system*: George 4

*Programming language used*: FORTRAN

*High speed store used*: 15 kwords

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, direct access files

*No. of cards in combined program and test deck*: 922

*CPC Library subprograms used (for data)*: *Cat. No.*: ACZF; *Title*: DATSTOR; *Ref. in CPC*: 18 (1979) 377.

*Keywords*: chemical reactions, rate coefficients, gas laser, plasma

*Nature of physical problem*
With the specific end in view to predicting the build-up of secondary chemical species in the discharge tube of gas lasers, REACS is a program designed to generate all chemical reactions which could take place in such a plasma tube. These reactions provide input to a further code PLASKEM which solves the ordinary differential equations which describe the time rate of change of the chemical species. Options exist in REACS for the generation of reactions involving electrons and negative and/or positive ions.

*Method of solution*
For each possible set of integer ratios $N_1:N_2: \ldots :N_m$ of the elemental constituents of the plasma (subject to input restrictions), the program generates the array $(N_1, \ldots, N_m)$.

The array $(N_1, \ldots, N_m)$ is split into all possible sets of three arrays, $(n_1^{(1)}, \ldots, n_m^{(1)}), \ldots, (n_1^{(3)}, \ldots, n_m^{(3)})$ which together add vectorially to $(N_1, \ldots, N_m)$, and represent the three possible initial or final neutral molecules in a reaction. Neutral molecule reactions are formed by pairing all distinct sets of 3-arrays originating from the same parent $(N_1, \ldots, N_m)$. Note that one or two of the arrays $\boldsymbol{n}^{(1)}$, $\boldsymbol{n}^{(2)}$ and $\boldsymbol{n}^{(3)}$ may be null.

Separate subroutines are written to generate from the neutral molecule reactions all types of reaction involving electrons, and negative and positive ions. In order to reject reactions involving molecules which are chemically unstable, a list of "allowed" molecules is provided as input to the code.

*Restrictions on the complexity of the problem*
The model does not take into account possible excitation of molecules during the reactions. Reactions involving cluster ions are not generated.

*Typical running time*
60 s on the ICL 1906A.

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# NUMERICAL MODELLING OF A CHEMICAL PLASMA
## II. PLASKEM: A program to predict the variation with time of the number densities of chemical species within a plasma

S.A. ROBERTS
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Received 9 October 1978; in revised form 19 June 1979

## PROGRAM SUMMARY

*Title of program*: PLASKEM

*Catalogue number*: ACZE

*Computer*: ICL 1906A; *Installation*: University of Leeds Computing Centre

*Operating System*: George 4

*Programming language used*: FORTRAN

*High speed store required*: 63 kwords

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter, direct access file

*No. of cards in combined program and test deck*: 1586

*CPC Library subprograms used (for data)*:

| *Cat. No.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ACZD | REACS | 18 (1979) 353 |
| ACZF | DATSTOR | 18 (1979) 377 |
| ACWX | BOLTZ | 11 (1976) 369 |

*Keywords*: plasma chemistry, laser discharge

*Nature of physical problem*
PLASKEM is a program to predict the variation with time of the number densities of the various chemical species contained within a plasma, with particular interest in the plasma contained in the discharge tube of gas lasers. The chemical reactions within the plasma may include neutral molecule–neutral molecule collisions as well as electron–molecule, electron–ion and molecule–ion collisions. The plasma is assumed initially to contain known fractions of primary species which react to form secondary species.

*Method of solution*
The time rates of change of the number densities of the chemical species are described by a set of coupled, nonlinear differential equations. One equation is required for each primary and each secondary species. An additional equation is required to account for changes in the effective electron temperature. The equations are solved by three alternative methods, (1) Runge–Kutta method, (2) initially by the Runge–Kutta method and subsequently by a modified Hamming predictor–corrector method, (3) Gear's method.

*Restrictions on the complexity of the problem*
The model used is a spatially independent one, reactions involving the container walls are neglected. The model assumes that the ambient gas temperature remains constant.

*Typical running time*
To solve 20 equations over a period of 300 ns on the ICL 1906A requires of the order of 50 s.

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# NUMERICAL MODELLING OF A CHEMICAL PLASMA

## III . DATSTOR: A program to create a data base containing information on rate coefficients of chemical reactions

S.A. ROBERTS
*Department of Computer Studies, The University, Leeds, UK*

Received 9 October 1978; in revised form 9 February 1979

## PROGRAM SUMMARY

*Title of program*: DATSTOR

*Catalogue number*: ACZF

*Computer*: ICL 1906A; *Installation*: University of Leeds Computing Centre

*Operation system*: George 4

*Programming language used*: FORTRAN

*High speed store used*: 46 kwords

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, direct-access files

*No. of cards in combined program and test deck*: 1511

*Keywords*: chemical reactions, rate coefficients, database, plasma, laser

*Nature of the physical problem*
DATSTOR is a program to create or update a permanent data base containing information relating to the rate coefficients of chemical reactions, and to create or update a corresponding directory which provides a means for searching the data base for information for any given reaction.

*Method of solution*
To each chemical reaction are associated four integers from which the reaction may be uniquely identified, and the address of the data base record at which the rate information for the reaction is stored. The data base directory is designed so that given any four integers the corresponding data base address may be rapidly found.

In the case of the program being used to update an existing data base, the old data base and directory are left unchanged, and a new data base and directory are created containing the data of the old data base as well as the current input data.

*Restrictions on the complexity of the problem*
The data base is designed to store three types of information, (1) a constant rate coefficient, (2) tables of rate coefficient vs. the chemical name of a particle which does not change during the chemical reaction, (3) tables of rate coefficients vs. effective electron temperature. Tables of rate coefficients vs. gas ambient temperature have not been included.

*Typical running time*
40 s

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# CALCULATION OF THE NUCLEATION AND GROWTH OF DEFECT CLUSTERS

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*Atomic Energy Board, Private Bag X256, Pretoria 0001, South Africa*

Received 12 March 1979; in revised form 10 May 1979

## PROGRAM SUMMARY

*Title of program*: Cluster 78

*Catalogue number*: ACUE

*Computer*: IBM 370 model 155; *Installation*: Atomic Energy Board, Pretoria, S. Africa

*Operating system*: OSMVT

*Programming language used*: FORTRAN IV

*High-speed storage required*: 250 k

*No. of bits in a word*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none (unless plotter off-line)

*Other peripherals used*: disc, line printer, plotter (optional)

*No. of cards in combined program and test desk*: 4125

*Keywords*: radiation physics, radiation damage, point defects, clusters, nucleation, growth, dislocation loops, voids, chemical rate equations, computation, numerical integration

*Nature of problem*
The program calculates the probability of interaction of point defects, defect clusters and gas atoms using chemical rate reaction theory [1,2]. The resulting set of differential equations is numerically integrated using a computer to give the number and size of the defect clusters as a function of irradiation time. The material is specified by listing certain constants and is applicable to elements and simple compounds.

*Method of solution*
The program is based on the subroutine of Gear [3], which integrates a set of ordinary differential equations by a step of length $H$. The trick is to keep $H$ as large as possible so that the program can be run to times equivalent to displacing each atom in the lattice one hundred times. $H$ is controlled by the subroutine [3] wherever possible. In certain cases, however, $H$ is set externally by extrapolation within the main program. Use of dimensionless quantities within the differential equations [2] enables one to overcome rounding-off errors, which are typical of this type of calculation.

Analytical solutions of the equations have not yet been found, apart from the one already published [4]. The output of the program is in a form which can be directly compared with experiment, i.e. the number and average size of the clusters as a function of the irradiation time.

*Typical running time*
To calculate the state of defect agglomeration to a dose equivalent to displacing each atom one hundred times takes typically between five and ten minutes.

*References*
[1] R.M. Mayer and L.M. Brown, to be published.
[2] R.M. Mayer and P.B. Kruger, Predictions of point defect agglomeration in nickel and copper during irradiation PEL-264 (Atomic Energy Board, Pretoria, 1979).
[3] C.W. Gear, Collected Algorithms from CACM, Algorithm 407; DIFSUB for solution of ordinary differential equations (1970).
[4] L.M. Brown, A. Kelly and R.M. Mayer, Phil. Mag. 14 (1969) 721.

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* Present address: Rupert International, P.O. Box 456, Stellenbosch 7600, South Africa.

** Present address: New Technology Division, BP Research Centre, Chertsey Road, Sunbury-on-Thames, Middlesex TW 16 7LN, UK.

Computer Physics Communications 18 (1979) 401–410
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# A PROGRAM TO CALCULATE INTERNAL CONVERSION COEFFICIENTS INCLUDING HIGHER-ORDER CORRECTIONS FOR ALL ATOMIC SHELLS

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*Zentralinstitut für Isotopen- und Strahlenforschung der Akademie der Wissenschaften der DDR, 705 Leipzig, Permoserstr. 15, GDR*

Received 21 February 1979; in revised form 13 July 1979

## PROGRAM SUMMARY

*Title of program*: INTERNAL CONVERSION COEFFICIENTS

*Catalogue number*: AAMB

*Computer*: ES 1040; *Installation*: Zentralinstitut für Isotopen- und Strahlenforschung

*Operating system*: OS/ES

*Programming language used*: FORTRAN IV

*High speed store required*: 282 Kbyte

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, printer

*No. of cards in combined program and test deck*: 1714

*Keywords*: nuclear physics, atomic physics, spectroscopy, atomic shell, internal conversion coefficient, electronic bridge, transition probability, gamma emission, Dirac equation

*Nature of the physical problem*
The internal conversion coefficients (ICC) including higher-order corrections are calculated for all atomic shells by solving the Dirac equation numerically for a given atomic potential.

*Method of solution*
The coupled radial Dirac equations are solved by inward–outward integration [1] for the discrete spectrum, and by outward integration for the continuum [2].

*Restrictions on the complexity of the problem*
The finite size of the nucleus (homogeneously charged sphere) is accounted for in the solution of the Dirac equation. However, contributions from inside the nucleus to the conversion matrix elements are neglected [3] as well as dynamic effects of the nuclear structure.

*Unusual features of the program*
In distinction from the program CATAR [4], which accounts for the dynamic effects of the nuclear structure as well as particle parameters, our program includes the calculation of the higher-order corrections for all atomic shells according to Krutov [5]. These corrections are discussed in more detail in ref. [6] and turn out to be relevant especially to the probability of the gamma emission.

*Typical running time*
The test case consisting of the subshell 3p1/2 of $^{99}\mathrm{Tc}^{\mathrm{m}}$ (2.17 keV; E3) requires 79 s to compile and 279 s to run on the ES 1040.

*References*

[1] M.E. Rose, Internal conversion coefficients (North-Holland, Amsterdam, 1958).
[2] L.A. Sliv and I.M. Band, in: Gamma-luči (Moskva-Leningrad, 1961).
[3] L.A. Borisoglebsky, E.M. Anderson, W.F. Trusov and G.S. Schuljakowsky, Tables of internal conversion of gamma-rays in outer atomic shells (Minsk, 1972) in Russian.
[4] H.C. Pauli and U. Raff, Comput. Phys. Commun. 9 (1975) 392.
[5] V.A. Krutov and V.N. Fomenko, Ann. Phys. (Leipzig) 21 (1968) 291.
[6] D. Hinneburg, M. Nagel and G. Brunner, Z. Phys. A., to be published.

Computer Physics Communications 18 (1979) 411–416
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# AN ALL-PURPOSE CURVE-FITTING PROGRAM FOR FUNCTIONS OF SEVERAL VARIABLES

E.D. von MEERWALL
*Department of Physics, The University of Akron, Akron, OH 44325, USA*

Received 20 July 1979

## PROGRAM SUMMARY

*Title of program*: UNIFIT4

*Catalogue number*: ABNH

*Computer*: IBM 370/158 AP; *Installation*: The University of Akron, Akron, OH 44325, USA

*Operating system*: OS/MVS

*Program language used*: FORTRAN IV (Gl)

*High-speed storage required*: $\geqslant$11000 words (45 kbt) without loader

*No. of bits in a word*: 32 (64 = double precision is used)

*Overlay structure*: none

*No. of tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 906

*Reference to other published version of this program*:
*Cat. no.*: ABMR; *Title*: UNIFIT2; *Ref. in CPC*: 11 (1976) 211

*Keywords*: general purpose, curve-fitting, least-squares, nonlinear, metric minimization, chi-square analysis, multi-dimensional

*Nature of physical problem*
The program fits theoretical models involving up to three independent variables ($x_1$, $x_2$, $k$), of arbitrary form, to data ($y$, $\Delta y$) and calculates chi-square.

*Method of solution*
A coarse grid-search and nonlinear metric minimization are used to minimize $\chi^2$, thereby optimizing up to 20 adjustable parameters. The gradient of $\chi^2$ is calculated by a finite-difference method. The program is an extension of an earlier published version [1].

*Restrictions on the complexity of the program*
The present limits of 20 parameters, and 200 data points, are easily extended.

*Typical running time*
On the IBM 370/158 III CPU, compilation takes about 8 CPU s; a typical 3–5 parameter fit to 100 data points takes about 4–8 s.

*Unusual features of the program*
To provide the most general and flexible curve-fitting facility,

(1) for each compilation the program may be set to fit any of several model types, for each of which the adjustable parameters may vary in number but must be the first several, the remainder serving as fixed constants;

(2) only the functions, but not their (analytic) derivative expressions, need to be supplied;

(3) the function expressions, and the data, may involve two continuous and one discrete (integer) independent variable;

(4) the fit procedure provides the chi-square of the goodness of fit, and the uncertainties in the fitted parameters.

*Reference*

[1] E.D. von Meerwall, Comput. Phys. Commun. 11 (1976) 211.

Computer Physics Communications 18 (1979) 417–426
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# A FORTRAN PROGRAM TO PERFORM SIGNAL AVERAGING, MULTICHANNEL SCALING, AND PULSE-HEIGHT ANALYSIS

E.D. von MEERWALL
*Physics Department, The University of Akron, Akron, OH 44325, USA*

Received 5 July 1979

## PROGRAM SUMMARY

*Title of program*: SAMCS1

*Catalogue number*: ABNG

*Computer* IBM 370/158AP; *Installation*: The University of Akron, Akron, OH 44325, USA

*Operating system*: OS/MVS

*Programming language used*: FORTRAN IV (G1)

*High-speed store required*: 20000 words (80 kbt) exclusive of loader

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, 132-column line printer

*No. of cards in combined program and test deck*: 828

*Keywords*: nuclear physics, spectroscopy, multichannel scaling, signal averaging, pulse-height analysis, data treatment, error analysis, regions of interest

*Nature of physical problem*
Most of the functions of multichannel scalers, signal averagers, and pulse-height analysis are to be performed, with significant enhancements, and a variety of data treatment options.

*Method of solution*
Standard data accumulation, calibration, interpolation, smoothing, and error analysis techniques are used; a plot is provided.

*Restrictions on the complexity of the program*
The present limits of 1024 for the dimension of the data arrays are easily extended.

*Typical running time*
On the IBM 370/158AP, the program compiles in about 8 CPU s; case processing time scales almost entirely with the amount of data supplied, since no extensive calculations are performed.

*Unusual features of the program*
(1) The program combines most of the functions of multichannel memory-based data acquisition devices of various kinds;
(2) it extends these functions to include, if appropriate, a per-pass scrutiny of abscissa calibration or offset and ordinate background level and slope, and the reproducibility from pass to pass;
(3) it perfomrs a first-order error analysis of the spectral channel contents, optional smoothing, and combinations of the two halves of memory;
(4) it provides a line-printer plot of processed and optionally transformed spectrum, ordinate uncertainties, and interpolation between channels.

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Computer Physics Communications 18 (1979) 427–440
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# COMPLEX ANGULAR MOMENTUM METHODS FOR ELASTIC SCATTERING WITH AN OPTICAL POTENTIAL

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*Department of Physics, University of Texas, Austin, TX 78712, USA*

and

H.H. WOLTER
*Sektion Physik, Universität München, D-8046 Garching, Fed. Rep. Germany*

Received 26 June 1979

## PROGRAM SUMMARY

*Title of program*: REGGE

*Catalogue number*: ABNF

*Computer*: CDC-6600; *Installation*: University of Texas Computer Center

*Operating system*: UT-2

*Programming language used*: FORTRAN IV

*High speed storage required*: 20992 words

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 1903

*Keywords*: nuclear, optical model, complex potential, complex angular momentum, analytic continuation, $S$-matrix, Regge pole, residue, background term, elastic scattering, Schrödinger equation, phase shifts, Sommerfeld–Watson transformation

*Nature of physical problem*
The computer program REGGE solves the radial part of the Schrödinger equation for a central complex potential. It locates the poles and zeros of the scattering $S$-matrix in a complex angular momentum plane, and also computes the residues of the poles. The pole terms thus obtained are combined with the background integral term and the sum, after being projected onto physical (real integer) angular momentum space, is used to calculate cross sections.

*Method of solution*
The radial Schrödinger equation is integrated by Milne's seven-point predictor–corrector method [1]. The $S$-matrix is determined by matching the solution to Coulomb wave functions of complex order [2]. The pole of the $S$-matrix is then searched by the Newton–Raphson method of iteration [3].

*Restrictions on the complexity of the problem*
(1) No negative energy is allowed.
(2) No more than 1000 integration steps in solving the differential equation are allowed.
(3) No spin–orbit interaction in the optical-model potential can be taken into account.
(4) No more than 90 partial waves of a real angular momentum are allowed.

*Typical running time*
Typical running time for calculating the $S$-matrix on the CDC-6600 with 600 integration steps per complex angular momentum is 0.23 s. The search times vary with distance from the initial values. The test cases TEST 1 and TEST 2 took 71 and 97 s, respectively.

*References*

[1] W.E. Milne, Am. Math. Monthly 40 (1933) 322.
[2] T. Takemasa, T. Tamura and H.H. Wolter, Comput. Phys. Commun. 17 (1979) 351.
[3] K.S. Kunz, Numerical analysis (McGraw-Hill, New York, 1957).

Computer Physics Communications 18 (1979) 441
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## ERRATUM NOTICE

| | |
|---|---|
| *Title of manuscript*: | A compact program of the SCF-X$\alpha$ scattered wave method |
| *Authors*: | S. Katsuki, P. Palting and S. Huzinaga |
| *Reference*: | Comput. Phys. Commun. 14 (1978) 13 |
| *Title of program*: | MSXALPHA |
| *Catalogue number*: | ACXN |

Computer Physics Communications 19 (1980) 51–61
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# IMPLEMENTATION OF THE PARTITIONED-DATA-SET CONCEPT FOR CDC COMPUTERS *

J.R. COMFORT **
*Kernfysisch Versneller Instituut, Groningen, the Netherlands*

Received 10 January 1979; in revised form 25 September 1979

## PROGRAM SUMMARY

*Title of program*: CDC PARTITIONED DATA SETS

*Catalogue number*: ACZQ

*Computer*: CYBER 74; *Installation*: Rekencentrum, Rijksuniversiteit te Groningen, Groningen, the Netherlands. Program has also run on CDC 6600 computers at Indiana University, Bloomington, Indiana and Los Alamos Scientific Laboratory, Los Alamos, New Mexico

*Operating system*: NOS/BE 1.2. Program has also run under SCOPE 3.4 and KRONOS 2.1

*Programming language used*: FORTRAN IV, EXTENDED and COMPASS

*High speed storage required*: 1874 words in subroutine package; main program requires 3185 words plus 8544 words for I/O buffers

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none required; at least one optional

*Other peripherals used*: Random-access devices such as disks and drums; line printer

*No. of cards in combined package*: 1220

*Keywords*: General purpose, utility, Partitioned data sets, disk organization, random/sequential I/O, libraries, card-image storage

*Nature of the physical problem*
Users' programs may need to make input/output to numerous sets of similar data, each to be read sequentially but in an order to be specified at execution time. It is convenient to group the sets of data into a single data set on a random-access device and arrange for the sequential transfer of the data for an individual "member". Documentary information and backup capacities may also be desired.

*Method of solution*
For CDC computers, a subroutine package implements a "partitioned data set" PDS concept [1]and provides linkages between users' Fortran programs and the CDC Record Manager I/O subroutines. For card-image applications, Program MANAGER is a handy utility program for data storage, retrieval and documentation.

*Restrictions on the complexity of the problem*
Users' programs must allocate core for PDS directories and file-information tables. I/O may be made with only one member of a PDS at a time. Record lengths are normally assumed to be of fixed length (shorter records are possible) with an upper limit of 32767 words. Program MANAGER is restricted to working with card-image data in alphanumeric coding (readable under alphanumeric format in FORTRAN). There may be no more than 500 members of a PDS.

*Unusual features of the program*
The CDS Record Manager subroutine and the DATE subroutine should be added to the test deck.

*References*

[1] J.R. Comfort, Computer Phys. Commun., this issue.

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* Work supported by the Stichting voor Fundamenteel Onderzoek der Materie (FOM).

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# ALGORITHM FOR THE FIRST ORDER HYDROSTATIC ELLIPTICITY OF A PLANET

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Received 4 July 1979

## PROGRAM SUMMARY

*Title of program*: HYDELP

*Catalogue number*: ACZT

*Computer*: IBM 3033

*Installation*: University of Toronto Computing Center

*Operating system*: OS

*Program language used*: FORTRAN IV

*High speed storage required*: 51 Kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 550

*Key words*: geophysics, hydrostatic ellipticity, figure of planet

*Nature of physical problem*
In geophysics the first order ellipticity of a planet is often required for a given model. In this new method the hydrostatic ellipticity of a planet can be calculated as a function of the mean radius. The input data needed are a set of values of the density of the planet as a function of the mean radius. The density model may have several jump discontinuities.

*Method of solution*
The density model (with or without jump discontinuities) is interpolated by cubic Hermite basis functions and the Darwin–de Sitter–Radau transformed first order ellipticity equation is integrated exactly to obtain the solution [1,2]. The numerical error is limited to that of the interpolation of the density model which is very small [3].

*Restrictions on the complexity of the problem*
As far as the theory is valid there are no known restrictions. The number of model points and the jump discontinuities may be set by users.

*Typical running time*
0.28 s for test run.

*References*

[1] E.C. Bullard, Monthly Notices, Geophys. Suppl. Roy. Soc. London 5 (1948) 186.
[2] H. Jeffreys, Geophys. J. Roy. Astr. Soc. 8 (1963) 196.
[3] W. Moon, Comput. Phys. Commun. 16 (1979) 273.

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Computer Physics Communications 19 (1980) 69–92
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# CALCULATION OF PHOTOEMISSION SPECTRA FOR SURFACES OF SOLIDS

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and

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*The Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK*

Received 15 July 1979

## PROGRAM SUMMARY

*Title of program*: PEOVER1

*Catalogue No.*: ACZY

*Computer*: IBM 370/165; *Installation*: Daresbury Laboratory, Daresbury, Warrington, Cheshire, UK

*Operating system*: OS

*Program language*: FORTRAN IV

*High speed storage required*: 240 Kbytes

*No. of bits per byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter

*No. of cards in program and test deck*: 4735

*Keywords*: photoemission, solid state, crystal, overlayer, surface, electron hole, multiple scattering

*Nature of problem*
To calculate the photoemission current as a function of the frequency, polarisation and direction of the electromagnetic radiation, and the energy and direction of the emitted electron from a single crystal surface possibly with ordered overlayers deposited on the surface.

*Method of solution*
The photoemission from a single atom is calculated to first order in the photon field. The initial and final state corrections are made by calculating the multiple scattering within and between the layers of the crystal [1]. The crystal is described by stacking identical layers of the bulk crystal and any overlayers that are required.

*Restrictions*
1) At present the programs assume that there is only one atom per unit cell in a given layer and that the bulk crystal is composed of a stack of identical layers.
2) If any overlayers are included then the lattice of atoms from each layer must be a (proper or improper) sublattice of the layer below. This is of course satisfied by the bulk crystal layers.

*Running time*
Approximately 10 s per point on the IBM 370/165 for the test run (T1).

*Unusual features*
All the arrays that have dimensions that depend on the input data are overlaid on a common block. The maximum sizes of the dimensions can then be increased simply by increasing the length of this common block.

*References*

[1] J.B. Pendry, Surface Sci. 57 (1976) 679.
J.B. Pendry, Low energy electron diffraction (Academic Press, London, 1974).

Computer Physics Communications 19 (1980) 93–101
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# A COMPUTER PROGRAM FOR DETERMINATION OF NUCLEAR PARAMETERS FROM INITIAL CONVERSION EXPERIMENTS

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Received 5 September 1979

## PROGRAM SUMMARY

*Title of program*: CFIT

*Catalogue number*: ABGS

*Computer*: IBM 370/135 and EC 1040; *Installations*: Institute of Information Theory and Automation, Prague, Czechoslovakia and Nuclear Research Institute, Řež near Prague, Czechoslovakia

*Operating systems*: OS/VS1 and OS/ES4.1M4

*Programming language used*: FORTRAN IV

*High speed store required*: 13 Kwords

*No. of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 824

*Keywords*: nuclear, atomic, internal conversion, electromagnetic transition, penetration effect, multipole mixture, least-squares method, experimental data, spectroscopy

*Nature of the physical problem*
The program analyzes the experimental data on gamma-ray internal conversion and determines the multipolarity mixing parameter and penetration parameter of the magnetic component for the nuclear electromagnetic transitions.

*Method of solution*
The best values of the parameters are found by the least-squares method. Due to the nonlinearity of the problem, the Gauss linearization method is used. The iterations are performed until the change in the least-squares sum is less than 0.1%. If this condition is not fulfilled within 100 iterations, the execution is terminated. All operations are performed using double precision.

*Restrictions on the complexity of the problem*
For a particular nuclear transition, a maximum of 25 experimental data items can be treated simultaneously. The program is not suitable for studying the hindered E1 transitions.

*Typical running time*
The running time depends mostly on the guess values of the parameters (given via input) and is typically 1 to 3 s per transition analyzed.

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# ASYPCK, A PROGRAM FOR CALCULATING ASYMPTOTIC SOLUTIONS OF THE COUPLED EQUATIONS OF ELECTRON COLLISION THEORY

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Received 10 July 1979

## PROGRAM SUMMARY

*Title of program*: ASYPCK

*Catalogue number*: AAJA

*Program obtainable from*: CPC Program Library, Queen's University of Belfast, Belfast, N. Ireland (see application form in this issue)

*Computer*: CDC 7600 (for test run); *Installation*: Univer of London Computer Centre, also tested on CDC 6600, CDC 6400, IBM 360/65, IBM 360/195, IBM 370/165 and CRAY-1

*Operating system*: scope 2.1.4 for test run

*Program language used*: FORTRAN IV

*High speed storage required*: 27 kwords (decimal)

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card-reader, line-printer, 2 permanent disc files, 1 scratch disc file, punch optional

*No. of cards in combined program and test deck*: 4046

*Card punching code*: CDC Standard Hollerith (BCD)

*CPC library subprograms used*:
*Catalogue number*: AAJB; *Title*: ASYPRO; *Ref. in CPC*: this paper, section 10

*Keywords*: atomic physics, asymptotic, solutions, electron–ion, electron–atom, electron–molecule, scattering, expansion methods, Fox–Goodwin integration

*Nature of the physical problem*
The program ASYPCK obtains solutions, at large radial distances, of the second-order differential equations of the type encountered in electron–ion and electron–atom scattering problems. ASYPCK can obtain either solutions at two radial points or solutions and their first derivatives at one point. Such solutions can be used as boundary solutions for a complete solution of a full set of close-coupling integro–differential equations encountered in electron collision problems (for example in the programs IMPACT [1] and RMATRX [2]). ASYPCK can also obtain sets of wave functions at a discrete mesh of radial points. These sets of functions can be used, for example, to obtain photo-ionization cross-sections and oscillator strengths [3].

*Method of solution*
For each reaction channel and associated boundary condition, the program obtains solutions at a point $r_f$ using an asymptotic expansion method (either the Burke and Schey expansion method [4] or the iterative WBK method of Norcross and Seaton [5]). These solutions are then inwardly integrated to obtain solutions at the desired radial distance. To overcome difficulties which can arise in the inward integrations, the Fox–Goodwin integration technique, described by Norcross and Seaton [6], has been included as an option.

*Restrictions on the complexity of the problem*
The program ASYPCK is provided in a form which must be pre-processed by a program ASYPRO (see section 10), which inserts dimensions and activates/deactivates machine dependent FORTRAN statements. The program ASYPCK is designed to work for both neutral atoms and ions and for both the cases of some channels open and all channels closed. Restrictions on the range of energies that can be handled are confined to a small range just below a threshold for neutrals and ions and also at a threshold for neutrals. The program can encounter difficulties in the cases where the channel energies are nearly degenerate or are very close to and above a threshold.

*Typical running time*

The running time depends on the problem being solved. The time increases approximately as $(\mathrm{NCHF})^2$ where NCHF is the number of free channels. The time also increases in cases where channel energies are nearly degenerate or close to a threshold. The time taken for the test run on the CDC 7600 at the University of London Computer Centre was 0.22 s.

*References*

[1] M.A. Crees, M.J. Seaton and P.M.H. Wilson, Comput. Phys. Commun. 15 (1978) 23.

[2] K.A. Berrington, P.G. Burke, M. Le Dourneuf, W.D. Robb, K.T. Taylor and Vo Ky Lan, Comput. Phys. Commun. 14 (1978) 367.

[3] H.E. Saraph, J. Phys. B 9 (1976) 2379

[4] P.G. Burke and H.M. Schey, Phys. Rev. 126 (1962) 147.

[5] D.W. Norcross and M.J. Seaton, J. Phys. B 2 (1969) 731.

[6] D.W. Norcross and M.J. Seaton, J. Phys. B 6 (1973) 614.

## PROGRAM SUMMARY

*Title of program*: ASYPRO

*Catalogue number*: AAJB

*Computer*: CDC 7600

*Installation*: University of London Computer Centre

*Operating System*: scope 2.1.4

*Programming Language*: FORTRAN IV

*High speed storage locations*: 4 kwords (decimal)

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card-reader, line-printer, one scratch file, 2 permanent disc files, punch file optional

*No. of cards in combined program and test deck*: 592

*Keywords*: atomic physics, pre-processor, editing, asymptotic, solutions, electron–ion, electron–atom, electron–molecule, scattering

*Nature of the physical problem*
ASYPRO is a pre-processor for the program ASYPCK (section 4, catalogue number AAJA).

*Method of solution*
ASYPRO reads two cards. The first specifies files IT1, IT2, IT3 and print level. File IT1 contains the unprocessed program ASYPCK and file IT2 is used for scratch storage. The processed FORTRAN program ASYPCK is written on file IT3. The second card specifies three basic dimension numbers for ASYPCK and a parameter MACH, which controls the activation or de-activation of machine-dependent statements in ASYPCK. ASYPRO computes subsidiary dimension numbers and, depending on the value of MACH, instructions for insertion or deletion of timing routines and the optional insertion of CDC PROGRAM cards. ASYPRO calls a modified version of the University College London String Replacement Program [1].

*Restrictions on the complexity of the problem*
ASYPRO uses one character not in the standard FORTRAN character set. In CDC Standard Hollerith this is a 5,8-hole punch and is printed on CDC machines as "$\leqslant$".

*Typical running time*
1.6 s on the CDC 7600 at the University of London Computer Centre for the processing of 3872 cards on file IT1.

*References*

[1] C. Day, Comput. Phys. Commun. 13 (1977) 101.

Computer Physics Communications 19 (1980) 139–157
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# EDITOR, A PROGRAM FOR AMENDING FILES OF CARD IMAGES

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Received 3 May 1978

## PROGRAM SUMMARY

*Title of program*: EDITOR

*Catalogue number*: ACZZ

*Computer*: CDC 7600; *Installation*: University of London Computer Centre

*Other machines on which program has been tested*: CDC 6400, CDC 6600, IBM 360/65, IBM 360/165, IBM 360/195

*Operating system*: SCOPE 2.1.4

*Programming language used*: FORTRAN IV

*High speed storage required*: 5 kwords (decimal)

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, 2 permanent disc files, up to 4 scratch files, card punch is optional

*Number of cards in combined program and test deck*: 917

*Keywords*: general purpose, utility, editing, machine-independent, files

*Nature of the problem*
It is quite common for the same program to be stored and run on a variety of computers, so that making alterations to a program may involve implementing the same changes on a number of machines. This can be both tedious and time consuming as it usual for different machines to have different file editing facilities, if any, forcing the user to produce a different set of updating instructions for each machine. EDITOR is a FORTRAN program written to overcome such problems by using machine independent instructions. Then, assuming that the original file is identical on all machines, the same instruction deck can be used for all machines.

*Method of solution*
EDITOR produces a corrected 'newfile' from an original 'oldfile' by reading, as data, instruction cards which identify cards to be deleted and positions for new cards to be inserted. New card images are read in as part of the instruction deck. EDITOR also has facilities for listing, punching and numbering parts or whole of a file.

*Restrictions on the complexity of the problem*
EDITOR has been designed to work on files of 80 character card images in which each card image has a unique identification in columns 73 to 80. The nature of the identification being a four-character identifier in columns 73 to 76 and a four digit number in columns 77 to 80 (i.e. exactly how CPC Library programs are identified). EDITOR can produce a file with such an identification trivially from a file not so numbered. There is no facility for amending part of a card image; if a change is to be made then the whole card image must be replaced.

*Typical running time*
The running time is almost completely determined by the size of the file being edited and not by the number of changes being made. Typically EDITOR takes 0.5 s to edit 1000 card images on the CDC 7600 at ULCC.

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# NUCLEAR DECAY SCHEME CONSTRUCTION BASED ON QUALITATIVE COINCIDENCES

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Received 18 January 1979; in revised form 3 September 1979

## PROGRAM SUMMARY

*Title of program*: ŠMUDLA

*Catalogue number*: AAPB

*Computer*: EC 1040; *Installation*: Nuclear Research Institute, Řež near Prague

*Operating system*: OS/ES 4.0M1-MVT

*Programming language used*: FORTRAN IV

*High speed storage required*: 270 000 bytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1579

*Keywords*: nuclear physics, spectroscopy, nuclear scheme, energy level, gamma transition, gamma coincidence

*Nature of the physical problem*

The program constructs possible variants of nuclear decay schemes from the knowledge of experimentally determined gamma transitions and their coincidences.

*Method of solution*

Coinciding transitions having their corresponding cross-overs are found. Afterwards more complex parts of decay scheme fragments with a given number of levels are constructed and they are tested for agreement with experimental information. The number of levels of the parts is gradually increased for as long as it is possible to find parts of a decay scheme conforming to experimental data. Fragments with the highest number of levels are finally printed in graphical form.

*Restriction on the complexity of the problem*

The program in its present form can process 300 transitions and 2000 coincidences and it constructs schemes with maximally 30 levels. These restrictions may be changed according to the computer memory. The range of working field needed for scheme building may be adjusted, too. However, for more complicated schemes results might be incomplete if the working field is too short, while the running time may considerably increase if the field is too large.

*Typical running time*

The running times vary considerably with the complexity of the resultant scheme. They range between a few seconds for less than 10 levels and two hours for more than 25 levels.

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# FOLDED YUKAWA-PLUS-EXPONENTIAL MODEL PES FOR NUCLEI WITH DIFFERENT CHARGE DENSITIES

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Received 1 October 1979

## PROGRAM SUMMARY

*Title of program*: FYPEDIFC

*Catalogue number*: ABQH

*Computer*: IBM 370/135; *Installation*: Central Institute of Physics

*Operating system*: DOS/VS-310

*Programming language used*: FORTRAN IV

*High speed storage required*: 118 kbyte

*Number of bits per byte*: 8

*Overlay structure*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 1359

*Keywords*: nuclear physics, structure, liquid–drop model, folded Yukawa-plus-exponential, fusion, fission, heavy ions, charge density asymmetry, potential energy surface

*Nature of the physical problem*
The deformation dependent terms of the potential energy in the folded Yukawa-plus-exponential model [1] for nuclei with different charge densities [2] are: volume, Coulomb and surface energies. They are expressed by an analytical relationship, two- and three-fold integrals, respectively, if one assumes nuclear shapes with axial symmetry. One has to consider separately the self-energies of the two fragments and their interaction energy.

*Method of solution*
For a given mass and charge asymmetry, the multiple integrals are computed numerically by Gauss–Legendre quadrature with $6 \times 6$ grid points, which are used to obtain by interpolation an array of $51 \times 51$ elements and to plot the potential-energy-surface (PES) map with the line printer. An iteration method is used by the saddle-point searching computer code.

*Restriction on the complexity of the problem*
The $4m \times 4m$ and $4m \times 4m \times n$ mesh points for numerical quadrature are chosen to assure the required accuracy for a given shape and charge density asymmetry. Only values $m, n \leqslant 64$ are allowed.

*Typical running time*
Typical running time for $n = m = 12$ and only one deformation set is 50 s. Variation of the running time with $n$ and $m$ is plotted in fig. 1.

*Unusual features of the program*
With few changes one can compute the gravitational energy instead of the Coulomb energy.

*References*

[1] H.J. Krappe, J.R. Nix and A.J. Sierk, Phys. Rev. Lett. 42 (1979) 215.
[2] D.N. Poenaru, M. Ivaşcu, D. Mazilu and A. Sandulescu, Rev. Roum. Phys., to be published.

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# P3M3DP – THE THREE-DIMENSIONAL PERIODIC PARTICLE-PARTICLE/ PARTICLE-MESH PROGRAM

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*Department of Computer Science, University of Reading, Whitenights, Reading, Berks., UK*

Received 11 July 1979

## PROGRAM SUMMARY

*Title of program*: P3M3DP

*Catalogue number*: ABVA

*Computer*: RL IBM 360/195

*Operating system*: OS-MVT

*Programming language used*: FORTRAN

*High speed storage required* **: 248 224 bytes

*No. of bits per word*: 32

*Overlay structure*: none

*No. of magnetic tapes required* ***: none

*Ohter peripherals used* ***: line printer

*No. of cards in combined program and test deck*: 7 695

*CPC library subprograms used*:

| *Catalogue number* | *Title* | *Ref. in CPC* |
|---|---|---|
| ABUF | OLYMPUS | 7 (1974) 245 |
| ABUA | FOUR67 | 2 (1971) 127 |

*Keywords*: PPPM, molecular dynamics, many body force calculation, three-dimensional, particle-particle/particle mesh ($P^3M$), ionic liquids, three-dimensional Vlasov gas, particle-mesh plasma simulation, many body gravitating system

*Nature of physical problems*
The program can be used to simulate many-body classical systems where interparticle forces are central and conservative. It is particularly effective for systems with rapidly varying short-range forces plus long-range Coulombic forces as is found in the simulation of ionic liquids or in the clustering of galaxies, although other systems, such as Lennard–Jones liquids and Vlasov plasmas can also be handled.

*Method of solution*
Interparticle forces are decomposed into spatially localised parts and approximately band limited parts. Accelerations are computed by using a direct particle-particle (PP) summation over the spatially localised forces and a particle-mesh (PM) method for the band limited forces. The equations of motion are approximated by the leapfrog scheme [1]. The resulting PPPM (or $P^3M$) algorithm [2] has the advantages that spatial resolution is not limited by mesh size as in PM schemes and cycle time is proportional to the number, $N_p$, of particles rather than $N_p^2$ as in a purely PP method with long-range forces.

*Restrictions on complexity of problem*
The implementation of the PPPM algorithm in this program is restricted to a triply periodic cubical computational box and a long-range force which is purely Coulombic.

*Typical running time*
The cpu time, $T$ (in seconds), on an IBM 360/195 for a single timestep is approximately (to within ≈10%) given by $T = (50 + 2N_n)\,10^{-5} N_p + \beta(N_g)$ where $N_n$ = number of particles in a sphere whose radius equals the range, $r_e$, of the short range force, $N_p$ is the number of particles and $\beta(N_g)$ is the time for solving the mesh equations ($\beta \approx 0.3$ for $N_g = 16$, 2.0 for $N_g = 32$ and 12 for $N_g = 64$). Typically, the program takes $1\frac{1}{2}$ s/1000 particles/timestep. $T$ includes the time for the dynamical calculation and the time for calculation of

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** This figure corresponds to the principal array core dimensioned to 7334.

*** For new runs with dummied graphics and no restart dumping.

pressure, temperature, internal energy and radial distribution function.

*Unusual features*
The program is written in standard FORTRAN using the OLYMPUS [3] conventions for structure, layout, notation and documentation. Graphical interface routines (the RDIPLT package) are included in documented dummy form so that potential users can include their own versions or obtain RDIPLT [4] when it is published.

*References*

[1] R.W. Hockney, Methods Comput. Phys. 9 (1970) 136.
[2] J.W. Eastwood, in: Computational methods in classical and quantum physics, ed. M.B. Hooper (Advance Publications, 1976) p. 206.
[3] K.V. Roberts, Comput. Phys. Commun. 7 (1974) 237.
[4] D.N. Lawrence, Comput. Phys. Commun., to be submitted.

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# A PROGRAM FOR CALCULATION OF THE REFLECTION AND TRANSMISSION OF ELECTRONS THROUGH A SURFACE POTENTIAL BARRIER *

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Received 19 September 1979

## PROGRAM SUMMARY

*Title of program*: ELECTRONS REFLECTED BY SURFACE

*Catalogue number*: ACKR

*Computer*: CDC6400; *Installation*: Stockholm Universities Computer Centre, S-104 50 Stockholm, Sweden

*Operating system*: NOS 1.3

*Programming language used*: FORTRAN IV

*High speed storage required*: 20864 words

*No. of magnetic tapes required:* none

*Other peripherals used:* line printer, card reader and punch

Other peripherals used: line printer, card reader and punch

*No. of cards in combined program and test deck*: 1623

*Keywords*: solid state physics, scattering, surface barrier, LEED

*Nature of physical problem*

The program calculates the reflection and transmission coefficients for an electron scattered by a surface barrier potential. It is intended to be used in a LEED calculation.

*Method of solution*

Solution of the Schrödinger equation.

*Restrictions on the complexity of the problem*

The program is designed to be used in the energy intervals $-40 < \hbar^2 k_z^2/(2m) < -0.01$ and $0.01 < \hbar^2 k_z^2/(2m) < 150$ eV, where $k_z$ is the wavevector component perpendicular to the surface.

*Typical running time*

The running time depends on $k_z$, in a typical run the average time is 0.5 s for each $k_z$.

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* Work supported by the Swedish Natural Science Research Council.

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## ERRATUM NOTICE

*Title of manuscript*: Program ACQN to calculate transport collision integrals adapted to run on IBM computers
*Authors*: P.D. Neufeld and R.A. Aziz
*Reference*: Comput. Phys. Commun. 3 (1972) 269
*Title of adaption*: ACQN ADAPTED FOR IBM 360/75
*Catalogue number*: ACQN
*Adaption number*: 0001

---

## ERRATUM NOTICE

*Title of manuscript*: A plotting package for visually comparing theoretical and experimental results.

*Authors*: J. Anderson, R.C. Beckwith, K.J.M. Moriarty and J.H. Tabor

*Reference*: Comput. Phys. Commun. 15 (1978) 437

*Title of adaptation*: POLAR PLOT AND IMPROVEMENTS

*Catalogue number*: AAUN

*Adaptation number*: 0001

Computer Physics Communications 19 (1980) 327–335
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# SUBROUTINES FOR THE EVALUATION OF EXCHANGE INTEGRALS IN THE IMPACT PARAMETER FORMULATION OF ATOMIC CHARGE TRANSFER COLLISIONS

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Received 8 June 1979 in revised form 14 August 1979

## PROGRAM SUMMARY

*Title of program*: IPEXMAT

*Catalogue number*: ACZU

*Computer*: IBM 370/165; *Installation*: Science Research Council, Daresbury Laboratory, Daresbury

*Operating system*: OS/MVT Release 21.7

*Programming language used*: FORTRAN IV

*High speed storage required*: 60 Kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 828

*CPC Library subprograms used (for data): Cat. No:* ACZV; *Title*: REXMAT; *Ref in CPC*: this paper

*Keywords*: atomic, charge transfer, exchange integrals, Fourier transform, impact parameter, collisions

*Nature of the physical problem*
A convenient description of atomic charge transfer collisions at moderate and high velocities is provided by the impact parameter formalism. Within this formalism it is advantageous to use a basis consisting of Slater-type orbitals which possess the virtue of having an appropriate asymptotic behaviour. This choice, however, leads to exchange integrals which are difficult to compute rapidly. The present collection of subroutines is designed to compute tables of these one-electron exchange integrals which may be used to obtain the matrix elements required in charge transfer calculations by interpolation.

*Method of solution*
The exchange matrix elements are evaluated using the Fourier transform reduction method suggested by Sin Fai Lam [1].

*Restrictions on the complexity of the problem*
The principal and orbital angular momentum quantum numbers defining the single particle orbitals on each centre are restricted to the ranges $n \leqslant 12$ and $l \leqslant 2$ in the present version of the code. Both restrictions may be relaxed by including further algebraic results.

*Typical running time*
The test run including compilation, required about 5 s on an IBM 370/165.

*Unusual features of the program*
The code REXMAT, written in the REDUCE2 language [2] and described in the following program summary, may be used to generate the algebraic results necessary to extend the range of quantum numbers (defining the orbitals on each centre of the exchange integrals) which the code is able to handle.

*References*

[1] L.T. Sin Fai Lam, Proc. Phys. Soc. 92 (1967) 67.
[2] A.C. Hearn, REDUCE2 User's Manual, Utah Computational Physics Group Memo No UCP-19 (March 1973).

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* Present address: Daresbury Laboratory, Daresbury, Warrington, Cheshire, UK.

## PROGRAM SUMMARY

*Title of program*: REXMAT

*Catalogue number*: ACZV

*Computer*: IBM 370/165; *Installation*: Science Research Council, Daresbury Laboratory, Daresbury, Cheshire

*Operating system*: OS/MVT Release 21.7

*Programming language used*: REDUCE2

*High speed storage required*: 540 Kbytes (depends on the results required)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 491

*Keywords*: atomic, charge transfer, exchange integrals, Fourier transform, impact parameter, REDUCE2, collisions, algebraic manipulation

*Nature of the physical problem*

The impact parameter description of atomic charge transfer collisions using Slater-type orbitals as basis functions requires the computation of two-centre one-electron exchange integrals. The program REXMAT is designed to perform part of the algebra necessary to obtain these integrals in the form of one-dimensional integrals which may easily be evaluated numerically.

*Method of solution*

The Fourier transform method suggested by Sin Fai Lam [1].

*Restrictions on the complexity of the problem*

Certain modifications to the code REXMAT will be necessary if orbital angular momenta greater than 3 are to be considered. Comment statements within the source deck contain suggestions for such extensions.

*Typical running time*

The test run required about 78 s of CPU time.

*Unusual features of the program*

The output from the program is produced in a form which can be incorporated either directly or with a minor amount of editing into the FORTRAN program IPEXMAT described in the previous program summary.

*References*

[1] L.T. Sin Fai Lam, Proc. Phys. Soc. 92 (1967) 67.

Computer Physics Communications 19 (1980) 337–357
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# A PROGRAM TO INTRODUCE LOCAL SYMMETRY IN AB-INITIO COMPUTATIONS OF MOLECULES: IBMOL-7

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Giorgio CASTIGLIONE
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Enrico CLEMENTI
*Soc. Montedison, Istituto Ricerche G. Donegani, Via del Lavoro 4, Novara, Italy*

Received 12 April 1978; in revised form 18 September 1979

## PROGRAM SUMMARY

*Title of the program*: IBMOL-7

*Catalogue number*: ACYY

*Computer for which the program is designed*: UNIVAC 1100/20 and 1106

*Computer*: UNIVAC 1100/20; *Installation*: Istituto Ricerche G. Donegani

*Operating system*: EXEC 8

*Programming language*: FORTRAN V

*High speed storage required*: 64323 words + the storage allocated used as work area during the sort and specified in the definition of file R$CORE (17920 words in the run reported as an example)

*No. of bits in a word*: 36

*Overlay structure*: yes

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, magnetic disk

*No. of cards in combined program and test deck*: 18476

*Key words*: symmetry, local symmetry, integral, molecular, ab initio computation

*Nature of physical problem*
In ab initio computations on large molecules many two-electron multi-centre integrals can be saved when groups of centre repeat in the molecule. A program is made to automatically detect and exploit such repetitions without using point group symmetry.

*Method of solution*
All the four-centre groups are virtually compared; a list of equivalent groups, and related geometrical transformations, precedes the evaluation of four-centre two-electron integrals.

*Typical running time*
Running time is strongly dependent on the dimensions of the molecules: in the Long write-up this dependence is analyzed in detail.

*Unusual features of the program*
The program uses sort subroutines, supplied by the UNIVAC system library: the link with sort must be modified when other machines and therefore other sort subroutines are used. UNIVAC FORTRAN V quarter-word handling function (FLD) are used: they can be translated, rather easily, into single byte instructions for IBM 360 or 370 series machines. Some functions needing information from the operating system require small assembler routines.

Computer Physics Communications 19 (1980) 359–375
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# EDWIN – A PROGRAM FOR CALCULATING INELASTIC MOLECULAR COLLISION CROSS SECTIONS USING THE EXPONENTIAL DISTORTED WAVE AND RELATED APPROXIMATE METHODS

G.G. BALINT-KURTI, J.H. van LENTHE *, R. SAKTREGER ** and L. ENO ***
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Received 1 October 1979

## PROGRAM SUMMARY

*Title of program*: EDWIN

*Catalogue number*: AAJC

*Computer*: IBM 360/195; *Installation*: Rutherford Laboratory, Chilton, Didcot, Oxfordshire OX11 0QY, UK

*Operating system*: IBM system/360 OS

*Programming language used*: FORTRAN

*High speed storage required*: 118 K

*No. of bits in a word*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: disc (optional)

*No. of cards in combined program and test deck*: 3477

*CPC Library subprograms used*: none

*References to other published version of this program*: none

*Key words*: inelastic scattering, cross sections, rotationally inelastic scattering, distorted wave, exponential distorted wave, Magnus method, exponential method, Schrödinger equation

*Nature of physical problems*
EDWIN calculates inelastic molecular cross sections for collisions between an atom and a rigid rotor molecule.

*Method of solution*
Four approximate methods are available as options, all based upon the distorted wave Born approximation. They are: the distorted wave Born method [1], the centrifugally decoupled distorted wave method [2] and their exponential or unitarised counterparts.
The diagonal channel wavefunctions are propagated from $R$ to $R + \delta R$ using the Magnus propagation method [3]. At large separations as semiclassical WKBJ form is used.
The contributions to the non-zero distorted wave integrals are accumulated for each propagation interval. By using a phase–amplitude representation of the channel wavefunctions, analytic expressions can be found for these contributions, while each propagation interval may contain many wavelengths without loss of accuracy in the integrals.

*Restrictions on the complexity of the problem*
The present program treats only atom–linear molecule rotational scattering, but it is reasonably simple to adopt it to other physical problems. There are some limits on the number of channels and the potential which can be easily extended. The potential should be provided as a Legendre polynomial expansion in the atom–molecule angle. Both the value and first derivative of the $R$-dependent part must be available.

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** Present address: Department of Meteorology, University of Reading, Reading RG6 2AU, UK
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*Typical running times*

These depends on the various accuracy criteria and the complexity of the problem. Very roughly, the running time goes up with the square of the number of rotational levels. A typical calculation (Ar–$N_2$, 768 K, 8 rotational levels, 18 total angular momentum values) using the CDEDW method with an accuracy of about 1% requires 3 min on the IBM 360/195.

*Unusual features of the program*

The program is designed around the use of arrays in blank common which are dynamically allocated and whose storage requirements are assigned during execution. In the present version the dynamical storage allocation has been replaced by a single parameter in the main program which the user can set to suit his needs.

*References*

[1] G.G. Balint-Kurti, in: International review of science, Phys. Chem. Ser. II, vol. 1, eds. A.D. Buckingham and C.A. Coulson (Butterworths, London, 1975).

[2] L. Eno and G.G. Balint-Kurti, Chem. Phys. 33 (1978) 435.

[3] D. Chang and J.C. Light, J. Chem. Phys. 50 (1969) 2517.

Computer Physics Communications 19 (1980) 377–393
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# NUMERICAL SOLUTIONS OF THE BOLTZMANN TRANSPORT EQUATION *

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Received 14 August 1979; in revised form 21 April 1980

## PROGRAM SUMMARY

*Title of program*: NOMAD

*Catalogue number* : ABVC

*Computer for which the program is designed and others on which it is operable*:
*Computer*: CDC 7600; *Installation*: Los Alamos Scientific Laboratory

*Operating system*: LTSS

*Programming language used*: FORTRAN IV

*High speed storage required*: 38356 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer, disk file input and output, large core memory

*No. of cards in combined program and test deck*: 1509

*Keywords*: Boltzmann transport equation, electron energy distribution, gas discharge lasers, atomic and molecular transport data

*Nature of physical problem*
The purpose of NOMAD is to calculate the distribution function of electrons accelerated by a dc electric field in a mixture of atomic or molecular gases. This distribution function is then convolved with elastic and inelastic cross sections to provide energy loss rates. The code is most frequently used to provide pumping rates for gas discharge lasers.

*Method of solution*
NOMAD solves the linear Boltzmann equation in a flux divergent form. It converts the one-dimensional electron energy axis into a discrete energy grid by finite differencing the respective electron energy gain and loss terms. The result is a finite set of coupled, linear differential equations which define the number density of electrons at each energy as a function of time. This matrix of densities is then evolved forward in time using an implicit back-substitution algorithm until a predetermined convergence criterion defining a steady state is achieved. Once the steady state energy distribution of electron number densities is determined, the elastic and inelastic energy gain and loss terms are used to calculate rates for the gas mixture, heavy particle number density, and electric field strength in question.

*Restrictions on the complexity of the problem*
The version of NOMAD published here is intended for use in situations where the ionization level is not so high that electron–electron (e–e) collisions will have an important impact on the electron energy distribution. Modifications to handle e–e collisions are discussed in ref. [1]. These modifications add significantly to the running time of the program.

It should be noted that NOMAD, following the work of Holstein [2], assumes that the two-term expansion of the Boltzmann equation in terms of spherical harmonics is adequate. It is beyond the scope of this work to discuss the ramifications of this limitation.

NOMAD assumes the computer core has been preset to zero.

*References*

[1] S.D. Rockwood, Phys. Rev. 8A (1973) 2348.
[2] T. Holstein, Phys. Rev. 70 (1946) 367.

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* Work performed under auspices of the US Department of Energy.

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# ERRATUM NOTICE

*Title of manuscript*: An expansion equation of state subroutine

*Author*: K. Morgan

*Reference*: Comput. Phys. Commun. 5 (1973) 64

*Title of program*: EOSEXP

*Catalogue number*: ACSA

Computer Physics Communications 20 (1980) 191–211
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# A PROGRAM TO EVALUATE CLOSED DIAGRAMS ALGEBRAICALLY FOR ANGULAR MOMENTUM COUPLED PRODUCT OPERATORS *

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and

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Received 19 February 1980

## PROGRAM SUMMARY

*Title of program*: CONTRACTION-JT-RECOUPLING

*Catalogue number*: AAAM

*Computer for which the program is designed and others on which it is operable*:

| *Computer*: | *Installation*: |
|---|---|
| IBM 360/65 | University of Rochester |
| IBM 3033 | Louisiana State University |
| DEC VAX-11/780 | University of Toronto |

*Operating system*: HASP/OSMVT, MVS/JES2, VAX/VMS

*Programming language used*: FORTRAN IV

*High speed storage required*: 31 Kwords (122 Kbytes)

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, printer, magnetic disks

*No. of cards in combined program and test deck*: 3491

*Keywords*: algebraic expressions, angular momentum recoupling, contraction, coupled product, excitation operators, Hamiltonian, many particle matrix elements, nuclear structure, Racah recoupling, scalar and configuration traces, second quantised spherical tensor of half integer rank, spectral distribution, statistical spectroscopy, Wick's theorem, 6*J*-symbol sum rules, 9*J*-symbol sum rules

*Nature of physical problem*
The many particle trace of a product operator, expressed in terms of angular-momentum coupled spherical tensor creation and annihilation operators, can be evaluated as the sum of the different ways or diagrams to contract all the single particle operators [1]. In the coupled representation, the process of contraction involves recouplings of angular momenta and this can be tedious. The program is constructed to perform algebraically the contractions and the associated angular momentum recouplings. The output are (algebraic) expressions which can be used either as analytical results or as input to a separate program, CONTRACTION-COMPILER [2], constructed to write a Fortran code to carry out the numerical calculations. The primary motivation of the project is derived from the need of scalar and configuration traces in nuclear structure problems using spectral distribution methods.

*Method of solution*
The form of each basic operator is first examined to see if, by rewriting it in different possible forms, the anticipated number of Racah recouplings can be minimized. The product operator is then recoupled into a standard angular momentum structure, the fan-shaped pattern. The pattern of contraction is read in from an input file produced, for example, by the CONTRACT-BASIC-DIAGRAM [3]. Before a pair of single-particle operators is contracted, they are brought into

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* Work supported in part by NSF of USA and NSERC of Canada.

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adjacent positions using standard Racah angular momentum recoupling rules. A list of $6J$-symbols, Kronecker deltas, phase and statistical weight factors is kept and updated at every stage. Whenever a variable becomes a purely dummy index of summation, the entire list of $6J$-symbols is scanned to see whether sum rules can be used to reduce the number of $6J$-symbols and summation variables to a minimum. When all the single particle operators are contracted, the remaining $6J$-symbols are scanned again for possible reduction by sum rules including those involving $9J$-symbols.

*Restrictions on the complexity of the problem*

The restrictions are basically the same as those imposed in CONTRACTION-BASIC-DIAGRAM [3]: the number of basic operators should be no more than 20, the total number of single-particle operators no more than 40. In addition, the total number of different variables, including those generated intermediately by the program, Kronecker deltas and $6J$-symbols must not exceed 100 at any one time and the number of $9J$-symbols no more than 20. These restrictions can be easily removed by extending the dimensions declared in the program. For a basic operator, the maximum number of creation and annihilation operators is restricted to be no more than two of each kind and, in the case of a basic operator made of two creation and two annihilation operators, the final angular-momentum rank of the basic operator must be a scalar.

*References*

[1] B.D. Chang and S.S.M. Wong, Nucl. Phys. A294 (1978) 19.

[2] B.D. Chang, J.P. Draayer and S.S.M. Wong, to be published.

[3] B.D. Chang and S.S.M. Wong, Computer Phys. Commun. 18 (1979) 35.

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# A PROGRAM TO CALCULATE THE EIGENFUNCTIONS OF THE RANDOM PHASE APPROXIMATION FOR TWO ELECTRON SYSTEMS

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*Department of Computing Science, The University of Glasgow, Glasgow, Scotland*

Received 9 October 1979

## PROGRAM SUMMARY

*Title of program*: RPA TWO ELECTRON EIGENFUNCTION

*Catalogue number*: AAJD

*Computer*: IBM 360/370; *Installation*: NUMAC, University of Newcastle upon Tyne, Newcastle, UK

*Operating system*: IBM OS

*Programming language used*: FORTRAN (double precision)

*Other package used*: NAG

*High speed storage required*: 122 Kwords

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 555

*Keywords*: random phase approximation, time-dependent Hartree–Fock theory, eigenfunction, eigenvalue, two electron system, Numerov, secant method

*Nature of physical problem*
Knowledge of the eigenfunctions and eigenvalues of the random phase approximation (RPA) [1] or time-dependent Hartree–Fock (TDHF) [2] theory is sufficient for calculations of one electron properties for closed shell systems correct to at least first order in correlation [3]. The eigenfunctions of two electron systems satisfy a pair of second order eigenvalue differential equations coupled by an integral term. These eigenfunctions, characterized by a principal quantum number $n$ and an angular momentum quantum number $l$, are evaluated by the program. The user need only specify $n,l$ and supply data for a Hartree–Fock ground state orbital.

*Method of solution*
The integral coupling term is replaced by an exchange term satisfying a third differential equation [4]. The resulting set of eigenvalue differential equations is solved by attempting to match forward and backward trial solutions; this leads to a nonlinear equation for the eigenvalue which is solved by the secant method. In case the NAG Library [5] is not available the specifications of the NAG routines used are given as comments at the end of the program.

*Restrictions on the complexity of the problem*
For very large principal quantum numbers some dimensions must be increased. However, in such cases the user is encouraged to derive a formula asymptotic in $n$, if possible, for the properties of interest rather than solve the eigenvalue problem. Also $l \neq 0$.

*Typical running time*
On the IBM 370/168 the eigenfunctions corresponding to a single $nl$ pair, are obtained in 2.6 s.

*References*

[1] D.J. Thouless, The quantum mechanics of many body systems (Academic Press, New York, 1961).
[2] A. Dalgarno and G.A. Victor, Proc. Roy. Soc. A291 (1966) 291.
[3] D.J. Rowe, Nucl. Phys. 80 (1966) 209.
[4] D.R. Hartree, The calculation of atomic structures (Pergamon, Oxford, 1957).
[5] NAG Mark 7 Fortran Library Manual; NAG Minimanual Mark 7, available from Numerical Algorithms Group, 7 Bamburg Rd, Oxford, England.

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# ENERGY EIGENVALUES AND BOUND–BOUND TRANSITIONS OF HYDROGEN ATOMS IN A MAGNETIC FIELD USING CYLINDRICAL BASIS FUNCTIONS

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Received 20 December 1979

## PROGRAM SUMMARY

*Title of program*: CPOLAR

*Catalogue number*: AAHK

*Computer*: CDC 7600; *Installation*: ULCC, University of London

*Operating system*: SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: LCM: 71 kwords, SCM: 6.2 kwords

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 1405

*Keywords*: magnetic field, hydrogen, eigenvalues, eigenvectors, energy, bound–bound transitions, oscillator strength, wavelength

*NAG library routines used*: (from the NAG6FLCM library) F01AEF, F01AGF, F02BEF, F01AHF, F01AFF

*Nature of the physical problem*
Calculates energy eigenvalues and corresponding eigenvectors of a hydrogen atom in a uniform static magnetic field and also determines the bound–bound transition probabilities, wavelengths and oscillator strengths. The wavefunctions are represented by a basis of cylindrical functions of the form
$\chi_{\beta\delta}^{(m,\pi)} = z^{\alpha}\rho^{\beta}\mathrm{e}^{-\delta r^2}\mathrm{e}^{im\phi}$.

*Method of solution*
All integrals are calculated analytically and the eigenvalues and eigenvectors are found using routines * from the NAG library [1]. The eigenvalues are calculated using the method of bisection and corresponding eigenvectors by inverse iteration [2].

*Restrictions on the complexity of the problem*
Only transitions involving the first two states for each parity and $m$ are considered, but the program requires only a simple modification to include more if desired. The dipole velocity formulation of the bound–bound transition probabilities is calculated only for $\Delta m = 0$ transitions i.e. only the $\nabla_0$ matrix element is calculated.

*Typical running time*
To calculate eigenvalues and eigenvectors of a basis consisting of 128 terms, for two different parity and $m$ sets, and all possible transitions between the first and second states of each of the two sets the dipole length and velocity formulations, takes about 20 s CPU time depending on how many eigenvalues are being calculated (a maximum of 10).

*References*

[1] NAG Mark 7 Fortran Library manual;
NAG Minimanual Mark 7, available from Numerical Algorithms Group, 7 Banbury Rd., Oxford, England.
[2] J.H. Wilkinson and C. Reinsch, Handbook for automatic computation, vol. II, Linear algebra (Springer-Verlag, Berlin, 1971).

* In case these routines are not available their specifications are given as comments at the end of the program.

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# CALCULATION OF LEED DIFFRACTED INTENSITIES

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and

C.G. KINNIBURGH
*Windscale and Calder Works, Sellafield, Cumbria CA20 1PG, UK*

Received 7 January 1980

## PROGRAM SUMMARY

*Title of program*: CAVLEED

*Catalogue number*: ABVB

*Computer*: IBM 370/165

*Installation*: Cambridge University Computer Laboratory

*Operating system*: OS MVT

*Programming language*: FORTRAN IV (IBM)

*High speed storage required*: 240 kbytes

*Number of bits per word*: 32

*Overlay structure*: none

*Number of magnetic tapes*: none

*Other peripherals used*: card reader, line printer

*Number of cards in program and test deck*: 4876

*Reference to any other published version of this program*: cf. J.B. Pendry, Low energy electron diffraction (Academic Press, 1974)

*Keywords*: solid state, electron diffraction, LEED, MEED, RHEED, surface structure, electron scattering, layer method, overlayer, muffin-tin, lattice sums, chain method, perturbation calculation, layer doubling

*Nature of the physical problem*
An electron diffraction experiment on a crystal surface provides a diffraction pattern which reflects the 2-dimensional periodicity of the surface, and also a record of the diffracted beam intensities as a function of incident beam energy and direction. This is compared with theoretical intensity curves calculated on the basis of trial models for the surface structure: a program to compute intensity curves for a wide range of surface models is presented here.

*Method of solution*
The surface region of the crystal is regarded as being made up of well separated atomic layers parallel to the surface, each containing up to two atoms per unit cell: the layers need not be coplanar. Muffin-tin atomic potentials are assumed, the electron scattering properties of each atom being described by a set of input phase shifts. Multiple scattering between the atoms within a layer is calculated using either direct summation [1] or the chain method [2]. Multiple scattering between layers is included by either the renormalised forward scattering perturbation method or the matrix doubling scheme [1], to give the wave amplitudes of diffracted beams at the surface.

*Restrictions on the nature of the problem*
Layers may contain either one or two atoms per unit cell. A periodic bulk layer stacking sequence is assumed, and overlayers with lattices simply related to the bulk may also be included. Dimensions of arrays are set up for 6 phase shifts and 21 beams.

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*References*

[1] J.B. Pendry, Low energy electron diffraction (Academic Press, New York, London, 1974).
[2] J.B. Pendry and P. Gard, J. Phys. C8 (1975) 2048.

Computer Physics Communications 20 (1980) 267–274
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# THIRD VERSION OF A PROGRAM FOR CALCULATING THE STATIC INTERACTION POTENTIAL BETWEEN AN ELECTRON AND A DIATOMIC MOLECULE

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*Centre de Mécanique Ondulatoire Appliquée, 23, rue du Maroc, 75019 Paris, France*

Received 23 May 1979

## PROGRAM SUMMARY

*Title of program*: ONE CENTRE STATIC POTENTIAL
*Catalogue number* ACZR
*Computer*: IBM 370/168; *Installation*: Centre Inter Régional de Calcul Electronique, Bâtiment 506, Campus d'Orsay, 91405 Orsay, France and Computer: IBM 370/158; *Installation*: Université de Liège, Belgium
*Operating system*: JES 3
*Program language*: FORTRAN IV
*High speed storage required*: 475 Kwords
*Number of bits in a word*: 32
*Overlay structure*: none
*Number of files requested*: 2 or 3
*Other peripherals used*: card reader, card punch, line printer
*Number of cards in combined program and test deck*: 2375
*Reference to other published version of this program*: *Catalogue number*: ACQW; *Title*: STATIC INTERACTION POTENTIAL; *Ref. in CPC*: 2 (1971), 261 and ACWO; *Title*: OCEP W.F. and STATIC POTENTIAL; *Ref. in CPC*: 11 (1976) 237
*Keywords*: quantum chemistry, single-centre expansion, static potential, dipole moment, quadrupole moment, multipole expansions, electron scattering

*Nature of the physical problem*
This program calculates the one-centre expansion of a two-centre wave function of a diatonic molecule and also the multipole expansion of its static interaction with a point charge. It is an extension to some classes of open-shell targets of the previous versions [1,2] and it provides both the wave function and the potential in a form suitable for use in an electron–molecule scattering program [3].

*Method of solution*
The original two-centre wave function is assumed to have a closed or restricted open-shell representation from a LCAO-MO-SCF calculation. The LCAO basis is of Slater-type centered on the two nuclei of the molecule: The atomic orbitals are expanded in Legrendre polynomials around either the centre of mass, or the centre of charge or one of the two atoms. The resulting wave function once orthonormalised by the symmetric orthonormalisation of Lowdin is used for calculating the static potential.

*Restrictions on the complexity of the problem*
This program is partially dynamically allocated either through an IBM 370/165 assembler subroutine or a main FORTRAN program (present version). The only restrictions are given below. Maximum number of basis functions is 50; the one centre expansion of the potential is limited to a maximum of 21 terms and the expansion of the molecular orbital is limited to 20 terms.

*Typical running time*
For 200 mesh points, 21 atomic and 4 molecular orbitrals, 15 terms in the expansion of the one-centre molecular orbital and 4 terms in the expansion of the static potential the program takes 42 s on an IBM 370/168.

*References*
[1] F.H.M. Faisal and A.L.V. Tench, Comput. Phys. Commun. 2 (1971) 261.
[2] F.A. Gianturco, Comput. Phys. Commun. 11 (1976) 237.
[3] G. Raşeev, Comput. Phys. Commun. 20 (1980) 275.

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# ELECTRON SCATTERING BY CLOSED OR OPEN SHELL DIATOMIC MOLECULES

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Received 23 May 1979

## PROGRAM SUMMARY

*Title of the program*: ELECTRON MOLECULE SCATTERING
*Catalogue number*: ACZS
*Computer*: IBM 370/168; *Installation*: Centre Inter Régional de Calcul Electronique, Bâtiment 506, Campus d'Orsay, 91405 Orsay, France and *Computer*: IBM 370/158; *Installation*: Université de Liège
*Operating system*: JES 3 and ASP
*Program language*: FORTRAN IV
*High speed storage requested*: with the test deck data: 640 Kwords
*Number of bits in a word*: 32
*Overlay structure*: none
*Number of files requested*: 4 or 5
*Other peripherals used*: card reader, card punch, line printer
*Number of cards in combined program and test deck*: 10 926
*CPC library subprogram required (for data)*:
*Cat. no.*: ACZR; *Title*: ONE CENTRE STATIC POTENTIAL; *Ref. in CPC*: 20 (1980) 000
*Reference to other published version of this program*:
*Cat. no.*: ACQO; *title*: ELECTRON MOLECULE SCATTERING; *Ref. in CPC*: 1 (1970) 445.
*Keywords*: quantum chemistry, electron scattering, open shells, single centre expansion, continuum Hartree–Fock, elastic cross sections

*Nature of the physical problem*
An extension of the existing low-energy electron diatomic scattering program [1] to open-shell molecular targets is presented. In this version, the orthogonalisation between bound and continuum orbitals is introduced. The $K$ matrix elements and the eigen-phases for rotational excitation are evaluated. The final continuum wave function is also calculated and stored on file.

*Method of solution*
The approach is based on a single-centre expansion of the molecular and incident electron orbitals. This centre can be any point for example the centre of mass, one of the atoms or the centre of charge of the molecule. The target molecule is represented by a LCAO–MO–SCF wave function which can be of closed or restricted open-shell type. It is assumed that the molecular axis does not rotate during the collision. The coupled integro–differential equations, with an orthogonalisation constraint and a modified exchange function (Raseev et al. [2]) are solved by a method analogous to the electron atom case [3].

*Restrictions on the complexity of the problem*
The program written in FORTRAN is dynamically allocated by an interface written in assembler (370/168). This interface can be replaced by a small FORTRAN main program provided with the program.

*Typical running time*
The test run of CH($^2\Sigma^+$($^1\Pi$ + e($\pi$))) with 200 mesh points which is about a half of the standard value requires about 23 s on an IBM 370/168. This test uses a five-term potential, has 6 compact exchange functions and performs the orthogonalisation with a 1$\pi$ orbital.

References

[1] A.L. Sinfailam, Comput. Phys. Commun. 1 (1970) 445.
[2] G. Raşeev, A. Giusti-Suzor and H. Lefèbvre-Brion, J. Phys. B 11 (1978) 2735.
[3] P.G. Burke and M.J. Seaton, Methods Comput. Phys. 10 (1971) 1.

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Computer Physics Communications 20 (1980) 291–307
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# A METHOD AND A PROGRAM FOR THE NUMERICAL EVALUATION OF THE HILBERT TRANSFORM OF A REAL FUNCTION

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Received 4 May 1979; in revised form 10 March 1980

In the first part of this paper a method for the evaluation of the Hilbert transform of a function, approximated by piecewise polynomials, is presented. In the second part a program is presented to be used when the function is approximated by cubic splines. We show that the Hilbert transform displays the same strong convergence properties as the cubic splines. The asymptotic properties of the Hilbert transform are shown to be very well reproduced.

## PROGRAM SUMMARY

*Title of the program*: FHT
*Cataloguenumber*: ABVD
*Computer*: IBM 370/155; *Installation*: UDAC, Uppsala Datacentral, Sweden
*Operating system*: OS/MVT
*Programming language used*: FORTRAN IV
*High speed storage required*: 3978 words
*No. of bits in a word*: 32
*Overlay structure*: none
*No. of magnetic tapes required*: none
*Other peripherals used*: card reader, line printer
*No. of cards in combined program and test deck*: 522
*Keywords*: Hilbert transform, general polynomial approximations, cubic splines

*Nature of the physical problem*
This program calculates the Hilbert transform of a continuous function. The evaluation of the matrix elements of the Green's function in quantum mechanics involves the evaluation of the Hilbert transform of the matrix elements of the Hamiltonian operator [1]. The same type of problem appears in many other fields of applied physics [1–5].

*Method of solution*
The program assumes that a cubic spline interpolation has been performed over the integration region. As the Hilbert transform function is evaluated at a point of the complex plane, the program checks first if the particular point needs special treatment. Then the corresponding analytical expressions for each interval are evaluated.

*Restriction on the complexity of the problem*
The function must be real and continuous over the integration interval. For complex functions two separate evaluation are necessary. In the appendix, it is shown how this program may be used in more general situations, for example when finite discontinuities are present.

*Typical running time*
The running time depends on the number of points included in the integration interval. For the test run this number was equal to 200. The evaluation of 60 different points of the complex plane took 11 s on a IBM 370/155.

*References*

- [1] E.N. Economou, Green's functions in quantum physics (Springer-Verlag, Berlin, Heidelberg, New York, 1979).
- [2] B. Velicky, S. Kirkpatrick and H. Ehrenreich, Phys. Rev. 175 (1968) 747.
- [3] K. Liebermann, B. Velicky and H. Ehrenreich, Bull. Am. Phys. Soc. 14 (1969) 320.
- [4] S. Kirkpatrick, B. Velicky and H. Ehrenreich, Phys. Rev. B1 (1970) 8.
- [5] P. Dennery and A. Krzywicki, Mathematics for physicists (Harper International Edition, New York, 1967).

Computer Physics Communications 20 (1980) 309–320
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# THE METHOD OF RAPTIS AND ALLISON WITH AUTOMATIC ERROR CONTROL

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Received 14 September 1979

## PROGRAM SUMMARY

*Title of program*: EXPFIT1
*Catalogue number*: AANA
*Computer*: IBM 370; *Installation*: NUMAC (Northumbrian Universities Multiple Access Computer)
*Operating system*: MTS
*Programming language*: FORTRAN IV
*High speed storage required*: 3675 words
*Number of bits in a word*: 32
*Overlay structure*: none
*Number of magnetic tapes*: none
*Other peripherals*: card reader, line printer
*Number of cards in combined program and test deck*: 763
*Keywords*: the method of Raptis and Allison, Schrödinger equation, classical turning point, numerical solution, second order differential equation, error control, phase shifts

*Nature of the physical problem*
Program EXPFIT1 solves the single channel radial Schrödinger equation in the form

$$y''(x) = \left[\frac{L(L+1)}{x^2} - E + V(x)\right] y(x) .$$

The test program solves the above problem for scattering of an electron by the static potential of atomic hydrogen, for a range of values of the energy $E$ and angular momentum $L$. The solution is calculated to a specified accuracy; scattering phase shifts are also calculated.

*Method of calculation*
The differential equation is solved by the method of Raptis and Allison [1] and the local truncation error is controlled as in Mohamed [2]. To calculate the phase shift the numerical solution in the asymptotic region is expressed as a linear combination of spherical Bessel functions.

*Restrictions on the complexity of the problem*
The restriction of the test program to the static potential of hydrogen may easily be removed by changing the function subprogram POT. The arrays F, XX which store the values of the solution and the corresponding mesh points may each store up to 8000 elements; the range of integration (which is specified by the user) and the values of the steplength chosen automatically by RAPAL may be such as to necessitate larger F and XX arrays but this can be easily arranged.

*Running time*
The test run which accompanies this paper took 4.8 s CPU time in a time-sharing environment; a separate compilation-only run took 3.3 s.

*Unusual features*
The steplengths used in solving the differential equation are chosen automatically by the program, in routine RAPAL, in accordance with a local accuracy criterion supplied by the user.

*References*

[1] J. Mohamed, Ph. D. Thesis, University of Durham (1979).
[2] A. Raptis and A.C. Allison, Comput. Phys. Commun. 14 (1978) 1.

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Computer Physics Communications 20 (1980) 337–347
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# CALCULATION OF THE VIRTUAL PHOTON SPECTRUM IN DISTORTED WAVE ANALYSIS *

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Received 5 September 1979

## PROGRAM SUMMARY

*Title of program*: VIRT SPEC

*Catalogue number*: ABPJ

*Computer*: IBM 370/158; *Installation*: Ohio University, Athens, OH 45701, USA

*Operating system*: VS1

*Programming language used*: FORTRAN IV

*High speed storage required*: 26 500 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: None

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1280

*Keywords*: virtual photon spectrum, distorted wave, electron scattering, Dirac–Coulomb

*Nature of the physical problem*
The virtual photon spectrum accompanying electrons or positrons scattering from a point charge $Z$ is calculated in plane wave Born approximation and in distorted wave Born approximation for E1, E2, E3 and M1 multipoles.

*Method of solution*
The radial integrals over Dirac–Coulomb functions and the spherical Hankel function are evaluated analytically using the techniques given in refs. [1–3]. The summation over partial waves is carried out by using the fact that matrix elements involving higher partial waves have very little Coulomb distortion effects and can be replaced by plane wave matrix elements which can be summed analytically.

*Restrictions on the complexity of the problem*
The present code is only valid in the point nucleus limit. Thus, the interpretation of experiments with lepton momenta such that there is appreciable nuclear penetration in terms of virtual photon spectra is open to question. See refs. [4,5] for a discussion of possible finite size effects on the plane wave virtual spectra. Also, the present code was programmed assuming relativistic leptons, $E_i \gtrsim 10$ m; and is not suitable for low energy muons except for photon energies well away from the end point. The restrictions on the allowed multipoles, E1, E2, E3 and M1 are only made for convenience, and can be relaxed by including additional analytic expressions in the subroutine PWAVE. Also, for storage purposes, only 30 different photon energies can be calculated with one set of data cards using the energy propagation. Of course, additional data cards can be used to propagate and calculate another 30 values.

*References*

[1] K. Sud, L.E. Wright and D.S. Onley, J. Math. Phys. 17 (1976) 2175.
[2] L.E. Wright, D.S. Onley and C.W. Soto Vargas, J. Phys. A10 (1977) 153.
[3] C.W. Soto Vargas, D.S. Onley and L.E. Wright, Nucl. Phys. A288 (1977) 45.
[4] W.C. Barber, Phys. Rev. 111 (1958) 1642.
[5] A.C. Schotter, J. Phys. G5 (1979) 371.

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* Supported in part by a grant from the US Department of Energy.

** Presently at Escuela de Física, Universidad de Costa Rica where partial support by CONICIT, Costa Rica is gratefully acknowledged.

Computer Physics Communications 20 (1980) 349–352
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# GILAT – RAUBENHEIMER METHOD FOR $k$ - SPACE INTEGRATION

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Received 12 December 1979

## PROGRAM SUMMARY

*Title of program*: GRINT
*Catalogue number*: AAPC
*Computer*: ICL 4-72; *Installation*: Czech Technical University, Prague
*Operating system*: MULTIJOB ICL 4-72
*Programming language used*: FORTRAN IV
*High speed storage used*: 22 kb for test run
*No. of bits in a byte*: 8
*Overlay structure*: none
*No. of tapes required*: none
*Other peripherals used*: card reader, line printer
*No. of cards in combined program and test deck*: 83
*Keywords*: $k$-space, density of states

*Nature of the physical problem*
Integrals over $k$-space which include a Dirac $\delta$-function may be calculated by this subroutine GRINT. The procedure represents the results (density of states, optical spectra, phonon spectra and other distribution functions) by means of a one-dimensional array DSF.

*Method of solution*
The $k$-space is divided into a large number of cubes. The integral over $k$-space is transformed to an integral over surfaces of constant energy, and in each of the small cubes the actual energy surface in the cube is replaced by a plane. Linear expansion of the energy around the cube centre using the gradient of energy at the cube centre is employed.

*Typical running time*
9 CPU (33 s) for the test run (GRINT is called $30^3$ times).

Computer Physics Communications 20 (1980) 353–371
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# MFP – A CODE FOR CALCULATING EQUATION OF STATE AND OPTICAL DATA FOR NOBLE GASES

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Received 26 November 1979; in final form 15 July 1980

## PROGRAM SUMMARY

*Title of program*: MFP

*Catalogue number*: ABVK

*Computer*: Univac 1110; *Installation*: MACC, University of Wisconsin, Madison, Wisconsin

*Operating system*: Univac 1110 EXEC VIII

*Programming language used*: standard FORTRAN

*High speed storage required*: 28 000 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 1477

*Keywords*: equations of state, radiation mean free paths, semi-classical

*Nature of the physical problem*
Optical and equation of state data are important to the solution of many problems in high temperature hydrodynamic phenomena. In particular, the propagation of a fireball through a gas is strongly dependent upon radiative transfer and the equation of state of the gas [1]. MFP is a code that computes ionization states and internal energies for gases. It also computes Rosseland and Planck averaged radiation mean free paths [2]. These quantities are computed on a three-dimensional grid of gas density, gas temperature and radiation blackbody temperature. Since transitions between molecular states are not included as radiation absorption mechanisms, data may only be generated for monatomic gases.

*Method of solution*
The ionization state is of primary importance to the optical behavior and the internal energy of gases. In MFP the average ionization state is calculated by using the Saha equation [3]. The densities of atoms in the six most common ionization states are determined by assuming that they are spread in a Gaussian about the average ionization state. These populations are subdivided into the lowest 20 excitation states by assuming that ions have hydrogenic energy levels and that the excitation states are in equilibrium at the gas temperature. The internal energy of the gas is taken as the sum of the kinetic energy of the ions, the kinetic energy of the ionized electrons, and the ionization energies of these electrons. A cross section for the attenuation of photons at a given energy by an atom in each of the 120 atomic states is calculated in the semi-classical approximation [4], where photo-ionization, inverse bremsstrahlung, Thomson scattering and atomic line absorption are considered as attenuation mechanisms. The absorption coefficient is the product of the attenuation cross section for each atomic state and the density of atoms in that state, summed over all of the states. Two different methods are used to average over the photon blackbody spectrum to obtain the Planck and Rosseland mean free paths. These quantities are output in machine readable tabulated form on a density, gas temperature, radiation temperature grid. A three-dimensional interpolation program is also included to access this data.

*Restrictions on the complexity of the problem*
At present the code MFP cannot generate a data table on a mesh larger than 17 density points by 20 gas temperature points by 20 radiation temperature points. In its present

form, MFP should not be used when the temperature is high while the density is low, because the Saha equation becomes inaccurate in this case [3]. These problems may be solved by future revisions of MFP. Care should be taken when chosing the widths of absorption lines as they can cause significant variations in the radiation mean free paths at low radiation temperatures. This shortcoming may be removed in a revision to MFP in which the line widths are explicitly calculated.

*Typical running time*
When run on the Univac 1110 at the Madison Academic Computing Center at the University of Wisconsin in Madison, Wisconsin, MFP uses approximately one second of CPU time for each choice of density, gas temperature and radiation temperature.

*Unusual features of the program*
MFP is written in standard FORTRAN [6] except for the use of the NAMELIST facility, through which parameters controlling the operation of the code may be modified. The program is written in a modular form which allows for easy changing of the physical content of the calculation. Included in the published version is a package of utility programs to be used in collecting and managing the large amount of data which can be generated by this code. The program PLOTTER, which provides graphics displays of the results of MFP, is not included in the published version because it may only be used on computers using the Univac graphic package GSP, but it is available from the authors on request.

*References*

[1] R.R. Peterson and G.A. Moses, University of Wisconsin Report UWFDM-315 (October 1979).
[2] Ya.B. Zel'dovich and Yu.P. Raizer, Physics of shock waves and high-temperature hydrodynamic phenomena (Academic Press, New York, 1967) ch. II.
[3] Ibid., ch. III.
[4] Ibid., ch. V.
[5] D. Mosher, NRL Memorandum Report 2563 (March 1973)
[6] Standard FORTRAN Programming Manual, Computer Standard Series (National Computer Centre, Manchester, England, 1970).

Computer Physics Communications 20 (1980) 373–412
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# COLASE – A $CO–N_2$–He LASER KINETICS CODE

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Received 18 February 1980; in revised form 18 July 1980

## PROGRAM SUMMARY

*Title of program*: COLASE

*Catalogue number*: ABVF

| *Computer* | *Installation* |
|---|---|
| Amdahl V/7 | Centre for Computer Studies, University of Leeds, Leeds, UK |
| CDC 7600 | UMRCC, University of Manchester, Manchester, UK |

*Operating system*: VM/CMS

*Programming language used*: FORTRAN IV

*High-speed store required*: 130 Kwords

*Number of bits in a word*: 48

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 2796

*Keywords*: laser, $CO-N_2$–He, e-beam, kinetics

*Nature of the physical problem*
From a knowledge of the rates of the various kinetic processes which occur in e-beam $CO-N_2$–He gas lasers, the code COLASE predicts the time history or, alternatively, the steady state values of the population inversion and hence the gain coefficients and output intensities for all lasing lines which are predicted to be above the lasing threshold.

*Method of solution*
A set of coupled, first-order, non-linear ordinary differential equations are developed which describe the time rate of change of the population number densities of the vibrational levels of CO and $N_2$, the light intensities for each lasing line and the ambient temperature of the gas. These equations are solved numerically using either Gear's method [1], or initially by the Runge-Kutta method and subsequently by a modified Hamming predictor–corrector method [2]. Alternatively, to simulate cw (steady-state) operation, an iterative method is used to solve the coupled, non-linear algebraic equations describing the cw population number densities and the light intensities.

*Restriction on program complexity*
The model assumes spatial homogeneity, that is effects of conduction and diffusion to the cavity walls are neglected.

*Typical running time*
In cw mode of operation, typically 10 s on the CDC 7600. In pulsed mode the run time is highly dependent on input parameters. Results for test case 1 took 70 s on the CDC 7600.

*References*

[1] C.W. Gear, Numerical initial value problems in ordinary differential equations (Prentice-Hall, London, Englewood Cliffs, 1971) ch. 9.
[2] A.R. Davies, K. Smith and R.M. Thomson, Comput. Phys. Commun. 10 (1975) 117.

Computer Physics Communications 20 (1980) 413–420
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# INJLOK – A $CO_2$ LASER INJECTION LOCKING CODE

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*Department of Computer Studies, The University, Leeds, UK*

Received 10 March 1980

## PROGRAM SUMMARY

*Title of adaption*: INJLOK

*Adaption number*: 0001

*Reference to original program*: *Cataloque number*: ACWD; *Title*: TLASER – a $CO_2$ laser kinetics code; *Ref. in CPC*: Comput. Phys. Commun. 10 (1975) 117

*Authors of original program*: A.R. Davies, K. Smith and R.M. Thomson

*Computer*: ICL 1960A, CDC 6600;

*Installation*: University of Leeds Computing Centre, University of London Computing Centre

*No. of bits in a word*: 48, 60

*No, of cards required to effect adaptation*: 398

*Additional keywords*: injection locking, mode selection, instantaneous frequency

*Nature of the physical problem*
The adapted code models the effect of an injected low-power frequency-stable signal on a high power $CO_2$ laser. The intensity and frequency of the output from the high-power laser is calculated.

*Method of solution*
The original program has been changed by substituting for the cavity field intensity equation, a set of equations describing the transient behaviour of the different mode field amplitudes and phases.

*Restrictions on the complexity of the problem*
The intensity of the injected signal is constant in time

*Typical running time*
For the test case provided the running time is 90 s on the Leeds 1960A and 16 s on the ULCC CDC 6600.

Computer Physics Communications 20 (1980) 421–428
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# HYMNIABLOCK – EIGENVALUE SOLVER FOR BLOCKED MATRICES

R. GRUBER

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Received 14 April 1980

## PROGRAM SUMMARY

*Title of program*: HYMBLO

*Catalogue number*: ABVI

*Computer*: CDC Cyber 7326, EPF Lausanne; *Operating system*: NOS BE

*Programming language used*: FORTRAN

*High speed store required*: 1541 + arrays

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: 3 disk files

*No. of cards in combined program and test deck*: 979

*Keywords*: General purpose, numerical mathematics, eigenvalue problem, inverse vector iteration, blocked matrix, symmetric matrix

*Nature of the problem*
Multidimensional stability problems lead to huge eigenvalue problems of the type $Ax = \lambda Bx$, which are only solvable when the matrix structures are not touched. In this package, $A$ and $B$ have block diagonal form.

*Method of solution*
The inverse vector iteration is used which converges towards the lowest eigenvalue in absolute value. By means of a shift of the spectrum it is possible to obtain any one of the modes. Decomposing $A$ first makes the iteration part much more efficient. The NEG facility gives the number of negative eigenvalues of the shifted problem and thus enables us to know which eigenvalue has been calculated.

*Restrictions of the complexity of the problem*
Both matrices, $A$ and $B$, have to be real symmetric and $B$ must be positive definite. Both must have the same block diagonal structure.

*Unusual features of the program*
The test program HYMBLO reads input data using NAMELIST which is not standard FORTRAN.

C-646

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# A PROGRAM TO SOLVE ROTATING PLASMA PROBLEMS

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and

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*FOM Instituut voor Atoom en Molecuulfysica, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands*

Received 17 September 1979

## PROGRAM SUMMARY

*Title of program*: PLASMA

*Catalogue number*: ABVE

*Computer*: Cyber 173-12; *Installation*: SARA (Stichting Academisch Rekencentrum Amsterdam), Amsterdam

*Operating system*: NOS/BE

*Programming language*: FORTRAN IV

*High speed storage locations*: 128 Kwords

*No. of bits in a word*: 60

*Overlay structure*: none

*Other peripherals used*: card reader, line printer, scratch disc store

*No. of cards in combined program and test deck*: 1072

*Keywords*: plasmadynamics, plasmacentrifuge, finite element method

*Nature of physical problem*
Rotation of a partially ionized gas in a cylinder, caused by crossed electric and magnetic fields.

*Method of solution*
The system of PDEs is discretized to a symmetric system of linear equations by means of the finite element method using continuous piecewise bilinear functions. The linear system is scaled and solved by means of the conjugate gradient method.

*Restrictions on program complexity*
A workspace is needed of about 16 times the dimension of the linear system to be solved. The maximal size of the workspace depends on the computer system.

*Running time*
Proportional to the square of the dimension of the linear problem.

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* Now at National Aerospace Laboratory NLR, Anthony Fokkerweg 2, 1059 CM Amsterdam.

Computer Physics Communications 20 (1980) 441–445
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# A PROGRAM FOR COMPUTING THE RIEMANN ZETA FUNCTION FOR COMPLEX ARGUMENT

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Ricardo Angel DEPINE *
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Received 4 February 1980

## PROGRAM SUMMARY

*Title of program*: RIEMANN ZETA FUNCTION

*Catalogue number*: ABVJ

*Computer*: IBM 360/50; *Installation*: Servicio de Computación en Salud, Universidad de Buenos Aires

*Operating system*: DOS

*Programming language used*: FORTRAN IV

*High speed store required*: 25 Kbytes

*No. of bits in a word*: 32

*Overlay structure*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 136

*Keywords*: Riemann Zeta function for complex argument, Fermi–Dirac function

*Nature of the physical problem*
The series expansion that gives a good approach to the Fermi–Dirac function $F_\sigma(\alpha)$ in the range $|\alpha| \approx 0$ requires the evaluation of the Zeta function $\zeta(s)$ for real argument [1]. However, important mathematical questions, concerning the location of the complex zeros of $\zeta(s)$ [2], lead us to construct a program directly applicable to complex values of the argument.

*Method of solution*
The method of solution is based on the series expansion of Gram [3] and Lindelöf [4], and other known results [2].

*Restrictions on the complexity of the problem*
The only restriction arises from the error in the values of the Bernoulli numbers [5].

*Typical running times*
Running times $\lesssim 1$ s.

*References*

[1] J. McDougall and E.C. Stoner, Phil. Trans. A267 (1938) 67.
[2] E.C. Titchmarsh, The theory of the Riemann Zeta function (Oxford University Press, Oxford, 1951).
[3] J.P. Gram, Acta Mathematica 27 (1903) 289.
[4] E. Lindelöf, Acta Mathematica 27 (1903) 305.
[5] M. Abramowitz and I. Stegun, Handbook of mathematical functions, with formulas, graphs and mathematical tables, 9th ed. (Dover, New York, 1972).

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* Fellow of CONICET.

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# COULOMB FUNCTIONS (NEGATIVE ENERGIES)

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Received 11 February 1980; in revised form 1 June 1980

## PROGRAM SUMMARY

*Title of program*: COULOMB FUNCTIONS (NEGATIVE ENERGIES)

*Catalogue number*: AANB

| *Computer* | *Installation* |
|---|---|
| IBM 370/165 | Daresbury S.R.C. Laboratory, Warrington, Lancs. |
| CRAY 1 | Daresbury S.R.C. Laboratory, Warrington, Lancs. |
| ICL 1906S | The Queen's University of Belfast, Belfast |

*Operating system*: OS/MVT RELEASE 21.7

*Programming language used*: ASA FORTRAN

*High speed storage required*: 90 000 bytes

*No. of bits in a word*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter for driver

*No. of cards in combined program and test deck*: 698

*Keywords*: atomic, reactions, scattering, wave function, Coulomb, Whittaker, Chebyshev, Runge–Kutta

*Nature of the physical problem*
The routine COUL calculates the exponentially decaying Whittaker functions $V_L(c, x)$ and their radial derivatives, where $c = \sqrt{-k^2}/Z$ and $x = Zr$, for real negative energy $k^2$ and for all $(c, x)$. It is well suited for all programs which require matching to asymptotic Coulomb wave functions in atomic physics.

*Method of solution*
The techniques employed are parameter dependent but rely heavily on the work of Curtis [1]. The Chebyshev approximation is used wherever possible, either to evaluate the function at the input values or to obtain values to enable numerical solution of the differential equation to occur. Recourse is also made to power series expansions. In general the $L = 0$ functions are first evaluated and then used to recur upwards in $L$ up to the input value.

*Restrictions on the complexity of the problem*
Routine COUL has been programmed for real values of $k^2$, $Z$ and $r$. $k^2$ must be a (non-zero) negative quantity, whilst $Z$ and $r$ must be real positive quantities.

*Typical running time*
Compile time using H-extended compiler 7.0 s; using G compiler 4.0 s. Execution of sample data 0.4 s (370/165).

*Reference*

[1] A.R. Curtis, Coulomb wave functions. Roy. Soc. Math. Tables, Vol. 11 (Univ. Press, Cambridge, 1964).

Computer Physics Communications 20 (1980) 459–460
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# ERRATUM NOTICE

*Title of manuscript:* Monte Carlo calculation of multiple scattering effects in thermal neutron scattering experiments

*Author:* J.R.D. Copley

*Reference:* Comput. Phys. Commun. 7 (1974) 289

*Title of program:* SLOW NEUTRON MULTIPLE SCATTERING

*Catalogue number:* ACIC

*Title of manuscript:* Monte Carlo calculation of multiple scattering effects in thermal neutron scattering experiments: modification to horizontal cylinder geometry

*Author:* J.R.D. Copley

*Reference:* Comput. Phys. Commun. 9 (1975) 64

*Title of adaptation:* HORIZONTAL CYLINDER GEOMETRY

*Catalogue number:* ACIC

*Adaptation number:* 0002

*Title of manuscript*: Calculation of wave-functions and collision matrix elements for one-electron diatomic molecules

*Author*: A. Salin

*Reference*: Comput. Phys. Commun. 14 (1978) 121

*Title of program*: MEDOC

*Catalogue number*: ACXY

C-650

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# ALAM, A PROGRAM FOR THE CALCULATION AND EXPANSION OF MOLECULAR CHARGE DENSITIES

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Received 20 June 1979; in revised form 29 January 1980

## PROGRAM SUMMARY

*Title of program*: ALAM

*Catalogue number*: ACZW

*Computer*: CDC 6000-7000 series; *Operating system*: KRONOS 2.1

*Programming language used*: FORTRAN IV

*High speed storage required*: 65000 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, disc

*No. of cards in combined program and test deck*:

*Keywords*: quantum chemistry, molecule, charge density, single-center expansion, scattering

*Nature of the physical problem*
The single-electron probability density function for a closed-shell linear diatomic or triatomic molecule is calculated from a single-configuration molecular-orbital wavefunction that is made up of nucleus-centered Slater-Type-Orbitals (STO's). The resulting function is expanded in Legendre polynomials in a single-centre coordinate system.

*Method of solution*
The nucleus-centred basis functions are transformed to single-centre coordinates, taking into account different conventions used in the definition of the nuclear geometry, spherical harmonics and molecular orbitals [1]. The expansion in Legendre polynomials is carried out by Gauss–Legendre quadrature [2]. Several user options are incorporated so as to avoid repetitive calculation of the charge density.

*Restrictions on the complexity of the problem*
No more than three nuclear centres can be accommodated. Only linear molecules (belonging to the point groups $D_{\infty h}$ or $C_{\infty v}$) are allowed. Other parameters, such as array lengths, can be adjusted by the user.

*Typical running time*
For the ground state of LiH, calculation of the charge density requires 0.38 s of CPU time. Each value of $a_\lambda(r)$ requires 0.01 s.

*References*

[1] M. Yoshimine and A.D. McLean, Intern. J. Quantum Chem. 1S (1973) 313.
A.C. Wahl, P.E. Cade and C.C.J. Roothan, J. Chem. Phys. 41 (1964) 2578.
S. Fraga and B.J. Ransil, J. Chem. Phys. 36 (1127) 1962.
[2] B. Carnahan, H.A. Luther and J.O. Wilkes, Applied numerical methods (Wiley, New York, 1969) section 2.10.

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Computer Physics Communications 21 (1980) 79–90
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# VLAM, A PROGRAM FOR COMPUTING THE ELECTRON–MOLECULE STATIC INTERACTION POTENTI FROM A LEGENDRE EXPANSION OF THE MOLECULAR CHARGE DENSITY

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Received 6 July 1979; in revised form 1 October 1979

## PROGRAM SUMMARY

*Title of program*: VLAM
*Catalogue number*: ACZX

*Computer*: CDC 6000–7000 Series; *Installation*: NOAA-ERL, Boulder, Colorado

*Operating system*: KRONOS 2.1

*Programming language used*: FORTRAN

*High speed store required*: $60\,000_8$ words *No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, disk, line printer

*No. of cards in combined program and test deck*: 1709

*Keywords*: molecular potential, electron–molecule collisions, interaction potential, quantum chemistry, scattering

*Nature of the physical problem*
Evaluation of the electron–molecule static interaction potential [1].

*Method of solution*
The procedure relies upon Legendre expansions of the Coulomb interaction between the incident electron and the target electrons and nuclei as well as upon a Legendre expansion of the molecular charge density itself.

*Restrictions on the complexity of the problem*
Restricted to systems with azimuthal symmetry.

*Typical running time*
Approximately 0.005 s/(radial point-moment) execution time for a run with several moments of the Legendre expansion. The test case took 4.191 s execution time for $\lambda = 0, 1, 2$ with a radial mesh of 241 points on a CDC 6600 computer. Timing is not expected to be very dependent upon the case.

*Reference*
[1] L.A. Collins and D. Norcross, Phys. Rev. A18 (1978) 467.

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* Member Quantum Physics Division, US National Bureau of Standards.

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# FOURIER ANALYSIS OF EXAFS DATA, A SELF-CONTAINED FORTRAN PROGRAM-PACKAGE

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Received 1 May 1980; in revised form 21 July 1980

## PROGRAM SUMMARY

*Titles of programs*: EXAFS 1, 2, 3, 4, 5

*Catalogue number*: ACUF

*Computer*: FELIX C-256; *Installation*: Computer Centre, Cluj-Napoca, Romania

*Operating systems*: SIRIS 2/3

*Programming language used*: FORTRAN IV

*High speed storage required*: 48, 48, 36, 36 and 54 kbytes

*No. of bits in a word*: 32

*Overlay structure*: none

*Other peripherals used*: card reader, line printer, disk file

*No. of cards in combined programs and test deck*: 1538

*Keywords*: spectroscopy, X-ray, absorption, scattering, solid state, local structure

*Nature of the physical problem*
The extended X-ray absorption fine structure (EXAFS), consists of the modulation of the absorption X-ray coefficient in the vicinity of the absorption edge that characterizes the elements in the material. Such modulation, called fine structure, is present because photoelectrons released from the X-ray absorbing atoms backscatter coherently from the neighbouring atoms [1].

Structural information obtainable by Fourier transform of the EXAFS function consists of bond distances, a measure of disorder in bond distances due both to thermal and structural disorder, coordination number, and chemical identity of the coordination shell [2].

The present program package performs the calculation of the normalized EXAFS data, the associated Fourier transform, and the best-fit values of the structural parameters for the first coordination shell.

*Method of solution*
The smoothing and the interpolation of the incident and transmitted X-ray intensity–energy function, is done by 3rd order polynomial functions and by Newton's interpolation formula for unequally spaced values of the argument [3]. The Fourier transform of the EXAFS function was performed by Filon's quadrature formulae [4]. The best fit values of structural parameters were computed by means of an iterative non-linear-parameters least-squares procedure [5].

*Restrictions on the complexity of the problem*
The maximum number of the absorption coefficient values in the present version is 500.

*Typical running time*
The time for the complete test case is 2 min.

*References*

[1] E.A. Stern, Phys. Rev. B10 (1974) 3027.
[2] E.A. Stern, D.E. Sayers and F.W. Lytle, Phys. Rev. B11 (1975) 4836.
[3] B.P. Demidovich and I.A. Maron, Computational mathematics (Mir Publishers, Moscow, 1973).
[4] M. Abramowitz and I.A. Stegun, Handbook of math. functions (Dover, New York, 1965).
[5] T.R. McCalla, Introduction to numerical methods and FORTRAN programming (Wiley, New York, 1967).

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# NEW VERSION OF PROGRAM FOR CALCULATING DIFFERENTIAL AND INTEGRAL CROSS SECTIONS FOR QUANTUM MECHANICAL SCATTERING PROBLEMS FROM REACTANCE OR TRANSITION MATRICES *

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Received 1 May 1980

## PROGRAM SUMMARY

*Title of program:* DCS2
*Catalogue number:* AAJE
*Computer:* Control Data Corporation Cyber 74 or 6600;
*Installation:* University Computer Center of the University of Minnesota
*Operating system:* KRONOS 2.1.2 or NOS 1.3
*Programming language used:* FORTRAN IV
*High speed store required:* $152400_8$ words as submitted but storage requirements depend on dimensions of arrays which may be changed for various applications *No. of bits in a word:* 60
*Overlay structure:* none
*Magnetic tapes and peripherals:* Depending on the problem and the options chosen, the program uses 2 to 5 files. The user may assign these to various combinations of card reader, line printer, tapes, and disk files
*No. of cards in combined program and test deck:* 2661
*Keywords:* atomic, nuclear, cross section, scattering, reactance matrix, transition matrix, scattering matrix, Racah coefficient, Clebsch–Gordan coefficient, differential cross sections

*Reference to other published versions of this program: Catalogue number:* ACRL; *Title:* DCS; *Ref. in CPC:* 5 (1973) 456; *Adaptation:* 0001; *Ref. in CPC:* 7 (1974) 172

*Nature of the physical problem*
This is a new version of the program [1] and adaptation [2] by Brandt et al. The storage requirements for a given problem have been reduced so that larger problems involving more coupled channels and higher angular momenta can be handled, and some convenient new options have been provided to simplify the input and choice of phase convention. In addition we corrected an error in the calculation of the opacity function and have added a calculation of the momentum-transfer cross section.

*Running time*
The two new test cases required 2.5 s and 34.1 s execution time, respectively, on the Cyber 74 computer.

*References*

[1] M.A. Brandt, D.G. Truhlar and R.L. Smith, Comput. Phys. Commun. 5 (1973) 456, 7 (1974) 177.
[2] M.A. Brandt, D.G. Truhlar and R.L. Smith, Comput. Phys. Commun. 7 (1974) 172.

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* Work supported in part by the National Science Foundation under grant no. CHE77-27415.
** Author to whom correspondence should be addressed.
*** Present address: Control Data Corporation, 1801 West Country Road B, Roseville, MN 55113, USA.

Computer Physics Communications 21 (1980) 109–118
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# A FORTRAN SUBROUTINE FOR THE BESSEL FUNCTION $J_n(x)$ OF ORDER 0 TO 10

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Received 9 June 1980

## PROGRAM SUMMARY

*Title of subroutine*: REALJN

*Catalogue number*: ABVM

*Computer*: IBM 370; *Installation*: NUMAC (Northumbrian Universities Multiple Access Computer)

*Operating system*: MTS

*Programming language*: FORTRAN IV

*High speed storage required*: 1900 words

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes*: none

*Other peripherals*: card reader, line printer

*Number of cards in combined program and test deck*: 625

*Keywords*: Bessel functions, Chebyshev series

*Nature of the problem*
The subroutine REALJN allows rapid calculation of the Bessel function $J_n(x)$ of real argument $x$ and integer order $n$, for $0 \leqslant n \leqslant 10$.

*Method of calculation*
The Bessel function is calculated by summing Chebyshev series, the coefficients of which are specified in DATA initialization statements within the subroutine. Separate Chebyshev series are used for the intervals $|x| \leqslant 8$ and $|x| > 8$, respectively.

*Restrictions on the complexity of the problem*
The order $n$ must be a positive integer from 0 to 10 inclusive. To permit other values of $n$ it would be necessary to provide the coefficients of the relevant Chebyshev series.

*Running time*
The execution time depends on the order $n$, on the required accuracy, and on whether or not the relevant value of $|x|$ exceeds 8. Times recorded range from about $7.8 \times 10^{-5}$ to $2.7 \times 10^{-4}$ s per subroutine call. More detailed information is given in the paper.

*Unusual features*
The subroutine REALJN allows the user to choose his own compromise between speed and accuracy in each subroutine call, either by specifying the number of terms to be retained in the Chebyshev series or by prescribing an upper bound on the acceptable truncation error.

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# GENERAL PURPOSE UNFOLDING PROGRAM LOUHI78 WITH LINEAR AND NONLINEAR REGULARIZATIONS

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Received 30 October 1979; in revised form 10 February 1980

## PROGRAM SUMMARY

*Title of program*: LOUHI78

*Catalogue number*: AAVD

*Computer*: UNIVAC 1108; *Installation*: Helsinki University of Technology, Helsinki, Finland

*Operating system*: EXEC8

*Programming language used*: FORTRAN IV

*High-speed store required*: 53200 words

*Number of bits in a word*: 36

*Overlay structure*: none

*Number of magnetic tapes*: none

*Other peripherals used*: card reader and line printer

*Number of cards in combined program and test deck*: 3227

*Keywords*: Fredholm integral equations, unfolding, activation measurement analysis, least squares method, regularization methods

*Nature of the physical problem*

Unfolding or deconvolution of the solution of Fredholm integral equations of the first kind is required in the interpretation of several physical measurements. Examples of such include neutron spectroscopy with activation detectors, moderating spheres or proton recoil measurements, and numerous others of analogous nature. The mathematical problem typically does not have a unique solution and in consequence prior knowledge of the solutions must be used by regularization or other methods to obtain physically meaningful solutions.

*Method of solution*

The unfolding problem is formulated as a generalized least squares problem whose objective function includes in addition to matching the measured data prior information of the smoothness, shape and magnitude of the solution, as available. These conditions are formulated either as a linear regularization problem which can be solved through fast matrix inversion techniques or a nonlinear regularization problem allowing also for logarithmic or relative weighting of the conditions and guaranteeing a nonnegative solution by using gradient minimization methods.

LOUHI78 is designed to be applicable to a large number of physical problems and to be extended to incorporate also other unfolding methods, such as parametric representation and linear programming techniques to make it a truly general purpose program offering a multitude of algorithms to choose and compare.

*Restriction on the complexity of the problem*

Designed primarily for the so-called few-channel problems the dimensions of the present version allow for up to 40 arguments and solution points.

*Typical running time*

Problems with 10 response functions and 40 solution points typically require about 4 s of UNIVAC 1108 cpu time with the faster linear method and about 15 s with the iterative nonlinear method.

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# ANALYSIS OF PHOTONUCLEAR YIELD CURVES BY THE VARIABLE BIN PENFOLD–LEISS METHOD

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Received 10 August 1979

## PROGRAM SUMMARY

*Title of program*: VBPL

*Catalogue number*: AAVC

*Computer*: CDC CYBER-73; *Installation*: University of Melbourne Computer Centre, Parkville, Victoria 3052, Australia

*Operating system or monitor*: Scope 3.4

*Programming language*: FORTRAN IV

*High speed store required*: none

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: disc, printer

*Number of cards in combined program and test deck: 1067* *

*Keywords*: photonuclear cross-section, matrix inversion, variable bin Penfold–Leiss

*Nature of the problem*
Various standard procedures have been evolved for the unfolding of photonuclear cross sections from a measured set of bremsstrahlung induced yield curves. These have been examined critically in ref. [1] which should be consulted for full details. This program uses the Variable Bin Penfold–Leiss (VBPL) method of matrix inversion to obtain a set of cross-section values each with its corresponding energy resolution. Various options are available. These include (1) conventional constant bin Penfold–Leiss analysis [2], (2) operator predetermined analysis bin width, variable with photon energy, (3) choice of X-ray spectrum [3] (presently either Schiff IOA or Bethe–Heitler) most appropriate for the X-ray convertor thicknesses used and the likely range of analysis bin widths, (4) provision for modification of the incident spectrum by absorption of the incident beam, both before and in the irradiated target, (5) the absolute calibration of the bremsstrahlung incident energy relative to the standard monitor ionization chamber, (6) the choice of presenting either the experimental yield data with corresponding X-ray monitor response for preliminary processing in the form of yield per unit monitor response, the so called reduced yield, or the presentation of the set of reduced yield data obtained from an alternative or external processing procedure.

*Method of solution*
Ref. [1], sections 2.1 and 4.3, should be consulted for the details of the matrix conversion procedure used. Selection of the analysis bin width can be made on the basis of the statistical criterion suggested by Thies [3]. This may proceed under automatic program control or subsequently by operator specification in order to minimize rapid changes of analysis bin width.

*Restrictions on the complexity of the problem*
The input data can consist of up to 230 yield points. The response function of the standard (P2) dose monitor is described by a polynomial of degree 5 or less; that of an experimental transmission dose chamber by a polynomial of degree 4 or less. If the user is specifying the analysis bin widths, up to 50 changes of these may be preselected. Absorption in the sample may be specified by absorption coefficients at up to 20 energy values.

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* Since some data cards use 80 columns, the overflow from columns 73–80 has been accommodated on a second card and should be repunched before use.

*Unusual features of the program*
The flexibility in selection of the analysis bin width allows the user to obtain optimum resolution in the analysed cross section consistent with the statistical quality of the input data at that stage over the full energy range.

*References*

[1] E. Bramanis, T.K. Deague, R.S. Hicks, R.J. Hughes, E.G. Muirhead, R.H. Sambell and R.J.J. Stewart, Nucl. Instr. and Meth. 100 (1972) 59.
[2] A.S. Penfold and J.E. Leiss, Phys. Rev. 114 (1959) 1332.
[3] H.W. Koch and J.W. Motz, Rev. Mod. Phys. 31 (1959) 920.
[4] H.H. Thies, Austr. J. Phys. 14 (1961) 174.

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# A PROGRAM FOR PERSPECTIVE VIEWS OF THREE-DIMENSIONAL SURFACES *

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and

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Received 31 July 1980

## PROGRAM SUMMARY

*Title of program*: TDPLOT3

*Catalogue number*: ABVL

*Computer*: IBM 370/165. IBM 360/75–370/155. *Installation*: TUCC, Research Triangle Park, NC 27709, USA. University of North Carolina Computation Center, Chapel Hill, NC 27514, USA

*Operating system*: OS/360, MVT Release 21-6

*Programming language used*: IBM FORTRAN H (code compatible with ANS FORTRAN except for minor extensions)

*High speed storage required*: Compilation 65 K words, link edit 30 K words, execution 50 K words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, CalComp plotter, Broomall plotter, or Tektronix 4013 storage oscilloscope

*No. of cards in combined program and test deck*: 2802

*Keywords*: three-dimensional surfaces, perspective projection, computer display, stereoscopy, cylindrical coordinates, polar coordinates, plotting, hidden-line removal

*Nature of the physical problem*
TDPLOT3 constructs either monoptic or stereoptic perspective projections of three-dimensional surfaces described in spherical-polar or cylindrical coordinates.

*Method of solution*
TDPLOT3 scales the surface so that its projection fits within specified plot dimensions. It then constructs the perspective projection [1] of the surface, determines, straightforwardly but efficiently, which points in the projection are hidden [2], and finally plots the projection with hidden lines removed.

*Restrictions on the complexity of the problem*
TDPLOT3 has been restricted to the display of surfaces $s(r, \theta)$ parametrized in spherical-polar or cylindrical coordinates where the radial, $r$, and angular, $\theta$, variables are both tabulated in uniform steps. The function $s(r, \theta)$ must assume only single, non-negative values at each $(r, \theta)$. No part of the display plane on which the surface is projected may lie within the domain of $s(r, \theta)$.

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* Research supported in part by the US Department of Energy and by the UNC Research Council.

*Unusual features of the program*

Hidden-line elimination is very efficient in TDPLOT3. It also features a cubic-interpolation routine which generates additional perspective points so that a smoother display of the surface may be constructed without needing additional input data or hidden-line search time. Monoptic and stereoptic views can be produced.

*References*

[1] I. Carblom and J. Paciorek, ACM Comput. Surv. 10 (1978) 465.

[2] I.E. Sutherland, R.F. Sproull and R.A. Schumacker, ACM Comput. Surv. 6 (1974) 1.

[3] H. Katzan, Jr., FORTRAN 77 (Van Nostrand Reinhold, New York, 1978).

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# ROOT-RATIONAL-FRACTION PACKAGE FOR EXACT CALCULATION OF VECTOR-COUPLING COEFFICIENTS

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Received 20 June 1980

## PROGRAM SUMMARY

*Title of program:* Root Rational Fraction Package
*Catalogue number:* ABVN
*Program obtainable from:* CPC Program Library, Queen's
*Computer: IBM 370/165*; *Installation:* University of Cambridge Computing Service
*Operating system:* HASP II / Phoenix
*Programming language used:* USANSI FORTRAN, Portable (PFORT) subset
*High-speed storage required:* about 7 Kwords overlaid, 10.5 K not overlaid
*Number of bits in a word:* 32
*Overlay structure:* IBM linkage editor statements supplied
*Number of magnetic tapes required:* none
*Other peripherals used:* none (except card-reader/printer or terminal)
*Number of cards in combined program and test deck:* 2153
*Keywords:* Vector coupling coefficients; Wigner 3*j*; Wigner 6*j*; Wigner 9*j*; power-of-prime arithmetic

*Nature of the physical problem*
A subroutine package is provided for the exact evaluation of vector coupling coefficients (Wigner 3*j*, 6*j* and 9*j* symbols) and for exact arithmetic involving these and related quantities. The main program supplied with the package can be used interactively like a calculator working in Reverse Polish Notation, to evaluate vector-coupling coefficients and to perform simple arithmetic on them.

*Method of solution*
The program uses power-of-prime arithmetic, with a list-processing technique which avoids arbitrary limits on the size of prime which can arise.

*Restrictions*
The program works in terms of numbers whose squares are rational fractions, and the only restriction is that all numbers which arise should be expressible in this form. In no problem investigated so far has this restriction caused any difficulty.

*Unusual features of the program*
The program is written in Ryder's Portable FORTRAN subset of USANSI FORTRAN, so that it should run without modification on most computers.

*Typical running time*
Calculation of a coupling coefficient takes a small fraction of a second. Extensive calculations involving sums and products of coupling coefficients, factorials etc. have been completed in a few seconds of IBM 360/165 cpu time.

Computer Physics Communications 21 (1980) 207–231
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# AN ATOMIC MULTICONFIGURATIONAL DIRAC–FOCK PACKAGE

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Received 18 February 1980; in revised form 1 August 1980

## PROGRAM SUMMARY

*Title of program*: MCDF

*Catalogue number*: AANC

*Computer*: IBM 360/195; *Installation*: Rutherford Laboratory, Chilton, Oxon

*Operating system*: OS/360, HASP

*Programming language used*: FORTRAN IV

*High speed storage required*: 344 kbytes if overlaid, 482 kbytes if not overlaid

*No. of bits in byte*: 8

*Overlay structure*: simple structure possible

*No. of magnetic tapes required*: one (alternatively permanent disc storage)

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 11 151

*CPC Library subprograms used*:
*Cat. no.*: AAHD; *Title*: NJSYM; *Ref. in CPC*: 8 (1974) 151
*Cat. no.*: ACRI; *Title*: CFPJJ-CFP in JJ COUPLING; *Ref. in CPC*: 4 (1972) 377

*Keywords*: atomic, multiconfiguration, Racah, fractional parentage, Dirac–Fock, recoupling coefficients, Slater integrals, complex atoms, relativistic, Dirac equation, wavefunction, *jj*-coupling, theoretical methods

*Nature of physical problem*
The relativistic Dirac–Fock equations are set up and solved numerically within the framework of the multiconfiguration approximation. This provides energy eigenvalues and orbital wavefunctions that can be used to calculate various atomic properties. For literature on methods see ref. [2].

*Method of solution*
Atomic state functions are constructed from a linear combination of configuration state functions which are eigenfunctions of $J^2$, $J_z$ and parity. These in turn are built from single-electron central field spinors. The self-consistent field approach results in coupled first-order differential equations for the orbital wavefunctions. These are solved iteratively using the method described by Desclaux, Mayers and O'Brien (program A of ref. [1]) within the context of various schemes for rendering the energy stationary.

*Restrictions on the complexity of the problem*
The present version of the program is restricted to 25 orbitals, 30 configurations with up to 350 grid points per orbital. These values may be increased by increasing the storage of the relevant arrays. The limit on the number of coefficients generated by the MCP package [2] is set at 500. Integrals of the form $I(ab)$ have been included in the Hamiltonian matrix but are not incorporated into the orbital equations. Code to force orthogonality of two orbitals with the same angular character

and identical occupation numbers has been included. This does not always result in a solution unless the system is near convergence; however, it is possible to set an option to relax this restriction, often resulting in approximately orthogonal orbitals which are then Schmidt orthogonalized.

*Typical running time*
Running time ranges from a few seconds for a small single configuration atom to about ten minutes for a many-configuration large atom, on an IBM 360/195. The four examples in the test deck took 149 s using the G-compiler and 47 s using the H extended plus compiler.

*Unusual features of the program*
The program includes useful features such as the recording of data set names, providing time and date of run, and the introduction of a timing scheme to save information on tape or disc if the program exceeds its cpu-time requests. These are implemented using local system routines which have been clearly indicated to allow the user to replace them if necessary. All routines use double precision arithmetic.

*References*

[1] J.P. Desclaux, D.F. Mayers and F. O'Brien, J. Phys. B4 (1971) 631.
[2] I.P. Grant, Comput. Phys. Commun. 14 (1978) 312.

Computer Physics Communications 21 (1980) 233–246
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# A PROGRAM TO CALCULATE TRANSVERSE BREIT AND QED CORRECTIONS TO ENERGY LEVELS IN A MULTICONFIGURATION DIRAC–FOCK ENVIRONMENT

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Received 18 February 1980; in revised form 14 August 1980

## PROGRAM SUMMARY

*Title of program*: MCBP/BENA

*Catalogue number*: AAND

*Computer*: IBM 360/195; *Installation*: OS/360, HASP

*Programming language used*: FORTRAN IV

*High speed storage required*: 346 kbytes (if overlaid)
616 kbytes (if not overlaid)

*No. of bits in byte*: 8

*Overlay structure*: simple structure possible

*No. of magnetic tapes required*: one (or direct access device)

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 2858

*CPC Library subprograms used*:

*Catalogue number*: AANC; *Title*: MCDF; *Ref. in CPC*: 21 (1980) 207

*Keywords*: atomic multiconfiguration, Racah, fractional parentage, Dirac–Fock, recoupling coefficients, Slater integrals, complex atoms, relativistic, Dirac equation, wavefunctions, *jj*-coupling, theoretical methods, Breit, transverse, Rydberg, QED, vacuum polarization, self-energy

*Nature of physical problem*
The program is an extension of, and is used in conjunction with, a multiconfigurational Dirac–Fock (MCDF) program already published [1]. This previous program solved the MCDF equations for an atomic system and dumped the solution (i.e. wavefunctions etc.) to tape or direct access device (hereafter referred to as disk). The present program is able to read this dump and supply corrections to the MCDF energy levels that result from including the transverse Breit operator [2] in first order perturbation, the second order vacuum polarization [3] and an approximate estimate of the self-energy operator. The program is designed to be incorporated into the previous program structure so that the present programs are called as subroutines of that system.

*Method of solution*
As described more fully in refs. [1,2] we construct atomic state functions (ASF) from a linear combination of configuration state functions (CSF) which are eigenfunctions of $J^2$, $J_z$ and parity. These in turn are built from single-electron central-field spinors that are solutions of the one-electron Dirac equation. In ref. [2] a method of reducing matrix elements of the transverse Breit operator to a sum of products of coefficients and radial integrals is described. Routines to calculate these coefficients were developed within the framework of the coefficient-calculating routines of ref. [1] and these coefficients are stored on a tape/disc file. These are later read and multiplied by the relevant radial integrals which are calculated by reasonably straightforward numerical integration techniques.

After all the matrix elements for the system have been calculated, they are added in turn to the zero-order Hamiltonian matrix elements (obtained from program of ref. [1]) and the matrix diagonalized. The difference in the resulting eigenvalues from those of the zero-order matrix gives the Breit correction to the energy levels.

The second-order vacuum polarization corrections are obtained using the methods described in ref. [3]; this provides an analytic potential, which is integrated over the electron density to give corrections to the orbital energies. The self-energy corrections are an approximate estimate based on interpolation among the hydrogenic results for various atomic numbers supplied by Mohr [4].

*Restrictions on the complexity of the problem*
The present version of the program is restricted to 25 orbitals and 30 configurations with up to 350 grid points per orbital. However, the structure of the program allows these values to be increased by replacement of the relevant common statements.

*Typical running time*
This varies widely from problem to problem but is usually less than 10 s on the IBM 360/195. The four examples in the test deck took 66 s using the G-compiler and 30 s using the H extended plus compiler.

*Unusual features of the program*
The program includes a few system routines for such things as recording the time and date of run and giving the names of data sets used. These, however, are clearly marked in the source as such and can be easily replaced by equivalent local routines.

*References*

[1] I.P. Grant, B.J. McKenzie, P.H. Norrington, D.F. Mayers and N.C. Pyper, Comput. Phys. Commun. 21 (1980) 207.
[2] I.P. Grant and B.J. McKenzie, J. Phys. B13 (1980) 2671.
[3] L.W. Fullerton and G.A. Rinker, Phys. Rev. A13 (1976) 1283.
[4] P.J. Mohr, Ann. Phys. 88 (1974) 52.

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# PROGRAMS FOR THE MOLECULAR DYNAMICS SIMULATION OF LIQUIDS: I. SPHERICAL MOLECULES WITH SHORT-RANGED INTERACTIONS

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Received 25 June 1980

## PROGRAM SUMMARY

*Title of program*: MDATOM

*Catalogue number*: ABVO

*Computer*: CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: SCOPE 2.1.5

*Programming language used*: FORTRAN IV

*High speed storage required*: 7380 words

*No. of bits in a word*: 60

*No. of magnetic tapes required*: none

*Other peripherals used*: lineprinter, cardreader, disk

*No. of cards in combined program and test deck*: 1126

*Keywords*: molecular dynamics, liquid simulation, Lennard-Jones fluid

*Nature of the physical problem*
Study of the thermodynamic, structural and dynamic properties of liquids or solids.

*Method of solution*
A system of a few hundred molecules is simulated. The equations of motion are solved in a series of time steps, at each of which the force on each molecule, due to its interaction with the other molecules in the system, is found. Periodic boundary conditions are applied to make the system pseudo-infinite. When the system is in thermal equilibrium thermodynamic measurements are made by averaging over time. The radial distribution function can be found, and also the mean square displacement of the molecules as a function of time. Information such as coordinates, forces and velocities at successive timesteps may be saved for further analysis.

*Restrictions on the complexity of the problem*
The present program is suitable only for a few hundred molecules with interactions described by central short-ranged pair potentials.

*Typical running time*
The execution time on the CDC 7600 per timestep of the simulation is 0.037 s with 108 particles, and 0.209 s with 256 particles. The complete test job, with compilation and execution for a total of 7000 timesteps, for 108 particles, took 260 s.

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# LATEN – A COMPLETE LATTICE ENERGY PROGRAM

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and

K.F. PRATT
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Received 30 August 1979; in revised form 16 September 1980

## PROGRAM SUMMARY

*Title of program*: LATEN

*Catalogue number*: ACMU

*Computer*: Burroughs 6700; *Installation*: Computer Centre, University of Warwick, Coventry, W. Midlands, CV4 7AL

*Operating system*: Master Control Program

*Programming language used*: FORTRAN IV

*High speed storage required*: 12 000 words (72 000 bytes) (average core usage)

*Number of bits in a word*: 48

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter and/or on line terminal; several random access formatted disk files are made during program execution

*Number of cards in combined program and test deck*: 3116

*Reference to other published versions of this program*: partly based on: A.B. Blake, QCPE 12 (1972) 222, and H.D.B. Jenkins and K.F. Pratt, Comput. Phys. Commun. 13 (1978) 341

*Keywords*: lattice energy, complex ion, Madelung constant, Bertaut method, electrostatic energy, repulsion energy, dispersion energy, basic radius, charge distribution, ionic salt

*Nature of the physical problem*
To calculate the lattice energy of an ionic salt (containing complex ions) by the most recently developed theory [1]; using as data crystal structure data, and minimising the energy with respect to the experimental unit cell constants.

*Method of solution*
The lattice energy is calculated using a 'term-by-term' equation and minimising the energy with respect to the unit cell lengths. For salts containing complex ions the calculations are performed throughout as a function of the charge distribution in the ions. The electrostatic contribution to the lattice energy is calculated using the Bertaut [2] approach (a version of the program MADELUNG DERIVATIVES (ACMO) [3] is employed), the repulsion term is calculated using the extended Huggins and Mayer [4] method and the dispersion term by adopting a London [5] approach.

*Restriction on the complexity of the problem*
The program (and implemented method) are designed primarily for the cases where *one* complex ion is present and a model for the repulsion calculations can be chosen involving a single sphere of 'unknown' radius. However, the program can be employed for all salts where a *full* experimental crystal structure is known and for which the ionic model can be assumed. Salts comprising unit cells possessing a permanent dipole moment cannot be treated by the Bertaut approach, and consequently cannot be considered for use with this program.

*References*

[1] H.D.B. Jenkins and K.F. Pratt, J. Chem. Soc. Faraday II 74 (1978) 968.
[2] E.F. Bertaut, J. Phys. Radium. 13 (1952) 499.
[3] H.D.B. Jenkins and K.F. Pratt, Comput. Phys. Commun. 13 (1978) 341.
[4] M.L. Huggins and J.E. Mayer, J. Chem. Phys. 1 (1933) 643.
[5] F. London, Z. Phys. Chem. (Leipzig) B11 (1930) 222.
[6] R.W.G. Wyckoff, Crystal structures, 2nd ed. (Interscience, New York, 1965).

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Computer Physics Communications 21 (1980) 271–277
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# A SPLINE-BASED METHOD FOR EXPERIMENTAL DATA DECONVOLUTION

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Received 27 August 1980

## PROGRAM SUMMARY

*Title of program*: DECONV

*Catalogue number*: ABVR

*Computer*: IBM 370/168; *Installation*: Bar-Ilan University Computer Center, Ramat-Gan, Israel

*Operating system*: OS/MVS

*Programming language used*: FORTRAN IV G

*High speed storage required*: 52 000 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1540

*Keywords*: deconvolution, unfolding, desmearing, resolution enhancement

*Nature of the physical problem*
In many types of experiments, notably in scattering and spectroscopic measurements of all kinds, the quantity or distribution $J(t)$ measured in the laboratory, can be expressed mathematically as a convolution of two functions:

$$J(t) = \int_{-\infty}^{\infty} K(s)\, J_0(t-s)\, \mathrm{d}s, \tag{1}$$

where $K(t)$ is the resolution (or response) function of the measuring instrument, and $J_0(t)$ is the same quantity as $J(t)$ but measured using an ideal instrument having infinite resolution [1]. The function $J_0(t)$ is, of course, the real information of interest. $K(t)$ is known either from measurements or through theoretical calculations.

Since in practice it is impossible to increase the resolution of an instrument past a given value, one must in general employ a deconvolution method to obtain $J_0(t)$ from the $J(t)$ and $K(t)$ data. Although eq. (1) can be formally solved by Fourier transform methods, a straightforward application of such methods without taking care of the random errors inevitably present in all experimental data, is doomed to failure [2,3]. Iterative methods [4] developed for solving eq. (1) are also very sensitive to the noise present in the $J(t)$ data, and are in general quite time consuming.

In reaction to this situation, we have developed a one-step deconvolution method, which does not suffer from the disadvantages mentioned above. It is simple to use, employs neither Fourier transforms nor iterations, and yields high accuracy results even in the presence of a high level of random experimental errors [5] in the $J(t)$ data. The present program is an implementation of our deconvolution method.

*Method of solution*
Let $J_0(t)$ be represented by a piece-wise cubic spline function [6]. Then, upon substitution of this function in (1), we obtain for $J(t)$ another piece-wise cubic spline, having the same knots, but different coefficients. These coefficients are related to those of the $J_0(t)$ spline via a set of equations [eq. (6) in the long write-up] involving the moments of the resolution function. These equations can be inverted to obtain the $J_0(t)$ spline coefficients in terms of the $J(t)$-spline coefficients. Thus, from fitting a piece-wise cubic spline to the $J(t)$ data, we directly obtain the coefficients of the spline function representing $J_0(t)$. This method, being a one-step procedure,

is fast and, due to the excellent smoothing properties of the spline function [7], it is insensitive to even large amplitude random errors in the $J(t)$ data.

*Restrictions on the complexity of the problem*
Only 250 $J(t)$ values can be treated by the present version in a single run.

*References*

[1] A. Guinier and G. Fournet, Small angle scattering of X-rays (John Wiley, New York, 1955).
[2] M. Wickham and S. Fornaca, Rev. Sci. Instr. 50 (1979) 747.
[3] Yu.A. Rolbin, L.A. Feigin and B.M. Shchederin, Sov. Phys. Crystallogr. 22 (1977) 663.
[4] J.A. Lake, Acta Cryst. 23 (1967) 191.
[5] M. Deutsch and I. Beniaminy, (1980) to be published.
[6] J.H. Ahlberg, E.N. Nielson and J.L. Walsh, The theory of splines and their application (Academic Press, New York, 1967).
[7] M.J.D. Powell, Report No. HL67/5309 (TP307) (1967), AERE, Harwell, Didcot, Oxon OX11 0RA, England.

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Computer Physics Communications 21 (1981) 315–322
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# A PROGRAM FOR COMPUTING THE FERMI–DIRAC FUNCTIONS

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Received 18 August 1980

## PROGRAM SUMMARY

*Title of program*: FERMI–DIRAC FUNCTIONS

*Catalogue number*: ABVP

*Computer*: IBM 360/50; *Installation*: Servicio de Computación en Salud, Universidad de Buenos Aires

*Operating system*: DOS

*Programming language used*: FORTRAN IV

*High speed store required*: 46055 bytes

*No. of cards in program*: 247

*Keywords*: Fermi–Dirac functions, statistical physics

*Nature of physical problem*
The Fermi–Dirac function appears in a wide range of physical applications. The package contains a function routine to calculate $F_\sigma(\alpha)$ for $\sigma > 0$ and all real $\alpha$.

*Method of solution*
The method of solution is based on the series expansions of Rhodes [1], Nordheim [2], McDougall and Stoner [3] and the authors [4].

*Restrictions on the complexity of the problem*
The relative accuracy parameter EPS should not be set below $10^{-5}$. The restriction is imposed in order to avoid a possible underflow condition. The user can improve the accuracy, depending on the computing system employed.

*Typical running times*
Running times are below 1 s.

*References*
[1] P. Rhodes, Proc. Roy. Soc. A204 (1950) 396.
[2] L. Nordheim, Müller Pouillets Lehrbuch der Physik, vol. 4 (Braunschweig, 1934) p. 4, as quoted in ref. [3].
[3] J. McDougall and E.C. Stoner, Phil. Trans. A267 (1938) 67.
[4] A. Banuelos, R.A. Depine and R.C. Mancini, J. Math. Phys. to be published.
[5] M. Abramowitz and I. Stegun, Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables (Dover, New York, 1972).

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Computer Physics Communications 21 (1981) 323–371
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# ERATO STABILITY CODE

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Received in final form 11 September 1980

## PROGRAM SUMMARY

*Title of program*: ERATO

*Catalogue number*: ABVS

*Computer*: CDC Cyber 170-720; *Installation*: Ecole Polytechnique Fédérale, Lausanne

*Operating system*: NOS BE

*Programming language used*: FORTRAN

*High speed store required*: 35 000 words

*Number of bits in a word*: 60

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer, disk files

*No. of cards in combined program and test deck*: 7901

*Keywords*: plasma physics, ideal MHD, variational principle, finite elements, spectrum, instabilities, eigenfunctions

*Nature of the physical problem*
This computer code treats the stability of a Tokamak-like plasma described by the ideal linearized magnetohydrodynamic (MHD) equations [1]. The plasma is considered to be in an equilibrium state. After perturbation of such an equilibrium, the evolution of the normal modes can be calculated by linearizing the ideal MHD equations. Any mode (unstable or stable) of the spectrum can be examined.

*Method of solution*
The variational form [2] of the 2D ideal MHD equations is treated by a finite hybrid element approach [3], which proves to be well suited to describe the features of the problem with sufficient accuracy [4]. The eigenvalue problem $\boldsymbol{Ax} = \omega^2 \boldsymbol{Bx}$ is solved by VEKIT (an inverse vector iteration), a subprogram of the block matrix library HYMNIABLOCK [5]. The code consists of 5 main programs (ERATO 1 to ERATO 5) linked together by disk files.

*Typical running time*
The running time is proportional to the number of poloidal flux surfaces $N_\Psi$, and to the cube of the number of angular intervals $N_\chi$ when $N_\chi > 20$. A typical case with 24 × 24 intervals in $\Psi$ and $\chi$ takes 15 min per eigenvalue on a CDC 6500.

*Unusual features of the program*
The code uses subroutines from two program libraries, the

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Present address: * IBM, Lausanne, Switzerland; ** General Atomic, San Diego, USA; *** Oak Ridge National Laboratory, USA; **** Zschokke SA Geneva, Switzerland.

utility routines of the CDC OLYMPUS package [6] and the eigenvalue package HYMNIABLOCK [5]. However, all the required subroutines are included in the ERATO package itself. ERATO is written in STANDARD FORTRAN [7], except for the use of the input facility NAMELIST which is available on most computers, and the CDC statement ENCODE which is used in ERATO 5. The plotting routines PLOTS, PLOT and SYMBOL used in ERATO 5 must be written to suit the local computer system and details of their arguments are given. ERATO also uses the CDC function subprogram DATE which picks up the actual date for plotting, and LOCF which gives the base address of an array. The programs ERATO 1–5 are arranged so that they can readily be combined into a single program if sufficient storage is available.

*References*

[1] B.B. Kadomtsev, Reviews of plasma physics, vol. 2 (Consultants Bureau, New York, 1966) p. 155.
[2] W.A. Newcomb, Ann. Phys. 10 (1960) 232.
[3] R. Gruber, J. Comput. Phys. 26 (1978) 379.
[4] R. Gruber and F. Troyon, 3ème Colloque Intern. Méthode de calcul scientifique et technique (Springer Verlag, Berlin, 1979); Lecture Notes Phys. 91 (1979) 288.
[5] R. Gruber, Comput. Phys. Commun. 20 (1980) 421.
[6] M.H. Hughes, K.V. Roberts and G.G. Lister, Comput. Phys. Commun. 10 (1975) 167.
[7] Standard FORTRAN Programming Manual, Computer Standard Series (National Computing Centre Ltd., Manchester, UK, 1970).

Computer Physics Communications 21 (1981) 373–383
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# SMOOS – A PROGRAM FOR THE FILTRATION OF NON-STATIONARY STATISTICAL SERIES

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Received 1 September 1980

A method is described for constructing numerical high and low frequency filters for the filtration of the trajectories of strongly non-stationary stochastic processes (e.g. with a trend of the type of resonance functions). Measures of function oscillations and function variability are introduced, and by making use of them the problem of constructing the above-mentioned filters is formulated in terms of the calculus of variations. A compact algorithm for the numerical implementation of the method is given and the corresponding standard FORTRAN-subroutines are described. A comparison with other filters is carried out.

## PROGRAM SUMMARY

*Title of program*: SMOOS, SMOSI

*Catalogue number*: ABVQ

*Computer*: CDC-6500; *Installation*: JINR, Laboratory of Computing Technique and Automation, Dubna

*Operating system*: SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: 1 kwords

*Number of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer, card reader

*No. of cards in combined program and test deck*: 237

*Keywords*: statistical series, non-stationary trend, numerical filter, difference equation, filtration, programming, data analysis

*Nature of the physical problem*
The program either smoothes a statistical series with a strongly non-stationary (e.g. resonance-like) trend or extracts from it a low frequency envelope from below.

*Method of solution*
The high and low frequency filters sought for, are constructed as solutions of the problem of minimization of oscillation or variability measures and distances of the functions from the initial series. The resulting difference equations are solved by a method, which is fast and compact with respect to the computer memory.

*Restrictions on the complexity of the problem*
None.

*Typical running time*
0.2 s for a series of 100 numbers.

Computer Physics Communications 21 (1981) 385–395
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# SIMULATION OF EPR-SPECTRA OF RANDOMLY ORIENTED SAMPLES

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Received 27 November 1979; in revised form 29 September 1980

## PROGRAM SUMMARY

*Title of program*: POWDER

*Catalogue number*: ABVG

*Computer*: CDC 6000; *Installation*: Rechenzentrum der ETHZ, 8052 Zürich, Switzerland

*Operating system*: SCOPE 3.4

*Programming language used*: FORTRAN IV G

*High speed storage required*: $130\,000_8$ words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, plotter, disk space

*No. of cards in combined program and test deck*: 826

*Keywords*: EPR, anisotropic *g*-tensor, anisotropic hyperfine-tensor, anisotropic perturbation calculation, numerical integration and differentiation, noise filter.

*Nature of the physical problem*
The EPR spectra of polycrystalline paramagnetic samples exhibits often complex features due to hyperfine and/or dipole–dipole and/or quadrupole interaction of the electronic and nuclear spins. This program calculates the first derivative of the EPR absorption spectrum of randomly oriented samples using the following approximations:

i) the eigenvalues of the spin Hamiltonian are given by second order perturbation theory;
ii) the intensities of the EPR transitions are determined by Zeeman interaction only;
iii) the paramagnetic species are uniformly or randomly distributed in space.
iv) "allowed" transitions ($\Delta M_I = 0$) are calculated only.

*Method of calculation*
The single crystal spectra for particular orientations are calculated. They are summed over all spacial orientations (Simpson rule) and convoluted with a line shape function giving the absorption line. A subsequent numerical derivation yields the 1st derivative spectrum and reduces the random deviations due to the limited number of orientations [1].

*Restriction on the complexity of the problem*
In the present version, the stick spectrum is convoluted with a lineshape function after the summation over all orientations has been carried out. This implies that only line widths independent upon orientation and $m_I$ can be treated. Furthermore, since a perturbation calculation is used, it is required that $\mathcal{H}$(Zeeman) > $\mathcal{H}$(hyperfine), $\mathcal{H}$(Zeeman) > $\mathcal{H}$(dipole–dipole) and that $\mathcal{H}$(hyperfine) > $\mathcal{H}$(quadrupole).

*Typical running time*
Ranges between 10 s and 10 min on the CDC 6000.

*References*

[1] B. Mohos et al., Anal. Chem. 48 (1976) 231; J. Chem. Phys. 60 (1974) 4633.

Computer Physics Communications 21 (1981) 397–406
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# A NUMERICAL CODE FOR THE PHASE-SPACE BOUNDARY INTEGRATION OF WATER BAG PLASMAS

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Received 15 December 1979; in revised form 23 September 1980

## PROGRAM SUMMARY

*Title of program*: PHASE SPACE BOUNDARY INTEGRATION

*Catalogue number*: ABVU

*Computer*: CDC 6600; *Installation*: Tel Aviv University, Israel

*Operating system*: Scope 3.3

*Programming language*: FORTRAN

*High speed store required*: CM 150 000 words

*No. of bits of word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: two

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 1450

*Keywords*: plasma physics, nonhomogeneous Vlasov systems, water bag plasmas

*Nature of the physical problem*
We consider the nonlinear evolution of nonhomogeneous Vlasov plasmas – a problem of great importance in both thermonuclear fusion research and astrophysics. In the past, only limited progress has been achieved in this direction, due to the complexity of the problem.

*Method of solution*
When the distribution function $f(x, v, t)$ of a collisionless plasma is pictured as the density of an incompressible "phase fluid" moving in the two dimensional $(x, v)$ phase space, by Liouville theorem, it is sufficient to follow the motion of the boundary curve(s) which enclose regions of constant $f$ in phase space in order to know the state of the system. Thus, it is possible to investigate a system consisting of a very large number of particles (enclosed by a boundary curve) without having to treat them explicitly. The method was first used by Roberts and Berk [1] for plasma systems. It has been further developed by Cuperman et al. [2] for gravitational systems. This paper describes the adaptation (transformation) of the improved phase-space boundary integration code of Cuperman et al. [2] to the plasma case.

*Restriction on the complexity of the problem*
The code may be used only for the investigation of one-dimensional (two-dimensional phase space), collisionless plasma systems consisting of regions of constant density (in phase space).

*Typical running time*
Execution times depend on the number of Eulerian strips used and on the number of mark points required to describe the system with the desired accuracy. Typically, if the number of Eulerian strips used is 215, the execution time per time step for one mark point is about $1.5 \times 10^{-3}$ s.

*References*

[1] K.V. Roberts and H.L. Berk, Phys. Fluids 10 (1967) 1595.
[2] S. Cuperman, A. Harten and M. Lecar, Astrophys. Space Sci. 13 (1971) 425.

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* Presently at the Courant Institute of Mathematical Sciences, New York University, New York, USA.

Computer Physics Communications 21 (1981) 407–419
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# CALCULATION OF (n, $\gamma$) CROSS-SECTIONS AND ASTROPHYSICAL REACTION RATES BY THE NUCLEAR STATISTICAL MODEL

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Received 22 September 1980

## PROGRAM SUMMARY

*Title of program*: HFNX

*Catalogue number*: ABVV

*Computer*: ICL 2980; *Installation*: Oxford University Computing Service

*Operating system*: VME/B

*Programming language used*: FORTRAN IV

*High speed storage required*: 16 Kwords

*No. of bits in a word*: 64

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader

*Cards in combined program and test deck*: 1038

*Keywords*: nuclear, astrophysics, reactions, low energy, statistical model, compound nucleus, giant dipole resonance, cross-sections, electromagnetic transitions, width fluctuation

*Nature of the physical problem*
Calculation of (n, $\gamma$) cross-sections for large numbers of target nuclei with $A > 50$ by the Hauser–Feshbach (HF) method. Calculation of astrophysical nuclear reaction rates, allowing for thermal population of excited states of the target.

*Method of solution*
Transition probabilities in the allowed decay modes of the compound nucleus are calculated (using level density functions wherever the final states are not experimentally identified), from values of neutron strength functions supplied to the program. The cross-sections are then calculated from the HF formula [1] modified by the width fluctuation correction [2]. The procedure is repeated for a set of incident energies, and again for such excited target states as are necessary; the (n, $\gamma$) cross-sections obtained are averaged over thermal populations of these states to give astrophysical reaction rates [3] at required temperatures.

*Restrictions on the complexity of the problem*
States with spins from 0 to 10, 1/2 to 21/2, can be included. Excited target states are not automatically provided within the program by a level density formula, and must be explicitly described to the program. E1, M1 and E2 electromagnetic transitions are included. E1 transitions are assumed to proceed through a giant dipole resonance [2]. Isotopic spin effects are not allowed for.

*Typical running time*
Depends on target spin, numbers of scattering and excited target states, and temperature range considered. For temperatures up to $3 \times 10^9$ K, in the most favourable case ($0^+$ target, no inelastic scattering or excited target states), typically 3 min on the OUCS ICL 2980.

*References*

[1] W. Hauser and H. Feshbach, Phys. Rev. 87 (1952) 366.
[2] J.E. Lynn, The theory of neutron resonance reactions (Oxford University Press, Oxford, 1968).
[3] D.D. Clayton, Principles of stellar evolution and nucleosynthesis (McGraw-Hill, New York, 1968).

Computer Physics Communications 21 (1981) 421–429
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# A FORTRAN PROGRAM TO FIT DIFFUSION MODELS TO FIELD-GRADIENT SPIN ECHO DATA

E.D. von MEERWALL and R.D. FERGUSON
*Physics Department, The University of Akron, Akron, OH 44325, USA*

Received 9 September 1980

## PROGRAM SUMMARY

*Title of the program*: DIFFUS5
*Catalogue number*: ABNI

*Computer*: IBM 370/158 AP; *Installation*: The University of Akron, Akron, OH 44325, USA

*Operating system*: OS/MVS

*Programming language*: FORTRAN IV (G1)

*High-speed store required*: 15 000 words (60 kbytes) without loader

*No. of bits in a word*: 32 (64 – double precision is used)

*Overlay structure*: none

*No. of tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1444

*Reference to earlier version of this program*:
*Cat. No.*: ABNE, *Title*: DIFFUS2, *Ref. in CPC*: 17 (1979) 309 (present program supersedes this earlier version)

*Key words*: diffusion, nuclear magnetic resonance, spin echo, magnetic field gradient method, curve fitting, restricted diffusion, anisotropic diffusion, multicomponent diffusion

*Nature of physical problem*
NMR spin echo attenuation in the presence of steady and/or pulsed magnetic field gradients is interpreted in terms of diffusion constants and parameters of inhomogeneity, anisotropy or relative intensity.

*Method of solution*
Least-squares curve fitting techniques are used to obtain two or three parameters of any of ten interpretive models to spin-echo attenuation data. Error analysis and plot are provided.

*Restrictions on program complexity*
The present limit of 50 data points per case is easily extended. Five types of experiment and ten types of interpretation are provided for. Program is designed for easy modification.

*Typical running time*
On the IBM 370/158 AP, the program compiles in about 19 s CPU; a case with 20 data points fitted with a restricted diffusion model takes up to 20 s CPU.

*Unusual features of the program*
1) Arbitrary diffusing nuclear species, and various experiment types with arbitrary steady and pulsed gradient magnitudes and timings are provided for;
2) Single and two-component diffusion, unattenuable echoes, spherically averaged anisotropic diffusion, and restricted diffusion with permeable or impermeable barriers are available in at least one modification each;
3) full error analysis gives uncertainties of all fitted parameters; chi-square permits checking the applicability of the model; a plot of data and fit is produced on the line printer.

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Computer Physics Communications 21 (1981) 431–436
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# MONTE CARLO CALCULATION OF MULTIPLE SCATTERING EFFECTS IN THERMAL NEUTRON SCATTERING EXPERIMENTS: IMPROVED COMPUTATION OF ELASTIC COHERENT SCATTERING INTENSITIES

J.R.D. COPLEY

*Institut Max van Laue-Paul Langevin, 156X Centre de tri, 38042 Grenoble Cédex, France, and Department of Physics, McMaster University, Hamilton, Ontario, Canada* *

Received 11 September 1980

## ADAPTATION SUMMARY

*Title of adaptation*: NEW ELSCAT SUBROUTINE

*Adaptation number*: 0003

*Reference to original program*:

*Catalogue number*: ACIC

*Title*: SLOW NEUTRON MULTIPLE SCATTERING

*Ref. in CPC*: 7 (1974) 289

*Author of original program*: J.R.D. Copley

*No. of cards required to effect adaptation (including directive cards)*: 517

*Nature of the physical problem*

This adaptation comprises a new version of the subroutine ELSCAT which is used to compute the differential cross-section for elastic coherent scattering into a detector. An analytical procedure is employed. The new subroutine is superior to the old one both in terms of accuracy and computing time.

Computer Physics Communications 21 (1981) 437
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## ERRATUM NOTICE

*Title of manuscript:* Alfven – A two-dimensional code based on SHASTA, solving the radiative, diffusive MHD equations

*Authors:* Wim J. Weber, J.P. Boris and J.H. Gardner

*Reference:* Comput. Phys. Commun. 16 (1979) 243

*Title of program:* ALFFYS

*Catalogue number:* ABUX

Computer Physics Communications 22 (1981) 13–31
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# PLATTSUM: A FORTRAN PROGRAM THAT EVALUATES ELECTROSTATIC LATTICE SUMS BY THE PLANEWISE SUMMATION METHOD

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Received 21 March 1980; in revised form 23 September 1980

## PROGRAM SUMMARY

*Title of the program*: PLATTSUM

*Catalogue number*: ABVL

*Computer*: IBM 370/158; *Installation*: Comisión Nacional de Energía Atómica, Av. del Libertador 8250, 1429 Buenos Aires, Argentina

*Operating system*: OS/VS1 or VM370/CMS

*Programming language used*: FORTRAN IV

*High speed storage required*: 67984 bytes

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer and/or on-line terminal

*No. of cards in combined program and test deck*: 1448

*Keywords*: lattice sums, crystal field, Lorentz factor, electrostatic crystal energy, Ewald potential, planewise summation method

*Nature of physical problem*
The calculation of the electrostatic potential due to a Bravais lattice of point charges presents several problems, of a practical as well as of a conceptual nature, coming from its convergence properties. Leaving aside the fact that the potential of an infinite charge distribution diverges (see ref. [1] and references therein for a discussion of this and related points), the numerical difficulties lie in the fact that the convergence of the sum is very slow.

*Method of solution*
We employ the planewise summation method (PSM), introduced by Nijboer and De Wette [2] and recently generalized by us [1]. The results given by this method correspond to a slab-shaped specimen. In this paper we program the equations given in refs. [1,3] for calculating the electrostatic potential of a point-charge lattice and its spatial derivatives up to the fourth order. In all cases in addition to the shape-dependent value of the sum a shape-independent result is obtained. The latter is used to improve the speed of the computation and to verify the correctness of the calculation (see section 2).

*Restriction on the complexity of the problem*
If the field point is very near to (without coinciding with) a lattice site the series given by the PSM have a very slow convergence. For this reason the program in its present form excludes points contained in a small parallelepiped centred at each lattice site ($\approx 10^{-4}$ of the unit cell volume). If a calculation at a point very near to a lattice site is needed the restriction can be relaxed (see section 5).
There are no restrictions on the complexity of the unit cell, i.e. on the crystal symmetry or the number of the sublattices.

*Unusual features of the program*
It allows one to calculate the electrostatic potential (and its derivatives up to the fourth order) in a perfect crystal made

of an arbitrary number of point-charge sublattices with arbitrary symmetry. It includes a method for a numerical check of the results.

*References*

[1] V. Massidda and J.A. Hernando, Physica 101B (1980) 159.
[2] B.R.A. Nijboer and F.W. de Wette, Physica 24 (1958) 422.
[3] F.W. de Wette and G.E. Schacher, Phys. Rev. 137 (1965) A78; errata: Phys. Rev. 138 (1965) AB4.

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# A PROGRAM GENERATOR FOR THE INCOMPLETE CHOLESKY CONJUGATE GRADIENT (ICCG) METHOD WITH A SYMMETRIZING PREPROCESSOR

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Received 6 March 1980

This paper is an extension of our previous paper "A program generator for the Incomplete LU-decomposition-Conjugate Gradient (ILUCG) method" which appeared in Computer Physics Communications. In that paper we presented a generator program which produced a code package to solve the system of equations $A\boldsymbol{x} = \boldsymbol{b}$, where $A$ is an arbitrary nonsingular matrix, by the ILUCG method. In the present paper we offer an alternative generator program which produces a code package applicable to the case where $A$ is symmetric and positive definite. The numerical algorithm used is the Incomplete Cholesky Conjugate Gradient (ICCG) method of Meijerink and Van der Vorst which executes approximately twice as fast per iteration as the ILUCG method. In addition, we provide an optional preprocessor to treat the case of a not diagonally dominant nonsymmetric and nonsingular matrix $A$ by solving the equation $A^{\mathrm{T}}A\boldsymbol{x} = A^{\mathrm{T}}\boldsymbol{b}$.

## PROGRAM SUMMARY

*Title of program*: GENIC

*Catalogue number*: ABSF

*Computer*: PDP-10/CYBER 172; *Installation*: Computer Center, Plasma Physics Laboratory, Princeton University, James Forestal Campus, P.O. Box 451, Princeton, NJ 08544, USA

*Operating system*: TOPS-10, version 6.03/NOS 1.3

*Programming language used*: FORTRAN

*High-speed storage required*: none

*Number of bits in a word*: 36 bits/60 bits

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: none

*Number of cards in combined program and test deck*: 3000

*Keywords*: linear sparse system, incomplete Cholesky, conjugate gradient, code generator

*Nature of the physical problem*
The program generator GENIC and the resultant Incomplete Cholesky Conjugate Gradient (ICCG) solver package SOLIC are applicable to a wide range of physical problems which require the solution of a large sparse system of linear equations:

$$A\boldsymbol{x} = \boldsymbol{b},$$

where $A$ is a symmetric and positive definite square matrix of rank $N$. It is also desirable that $A$ be reasonably diagonally dominant; that is, $A_{ii} \geqslant \Sigma_{i \neq j}^{N} |A_{ij}|$, for otherwise the incomplete decomposition used here may be a poor approximation of the complete decomposition and in the worst case the decomposition itself may become unstable. Since this is an iterative method, it is particularly suitable for large systems. The package is most efficient when the nonzero elements of $A$ appear clustered in diagonal bands. Such patterns are often found in implicit finite difference formulations of partial differential equations resulting from modeling of multidimensional physical problems.

*Method of solution*
For symmetric, positive definite matrices, the Incomplete Cholesky Conjugate Gradient (ICCG) algorithm of Meijerink and Van der Vorst [2] is used. For nonsymmetric matrices which are not diagonally dominant, a symmetrizing preprocessor is generated which transforms $A\boldsymbol{x} = \boldsymbol{b}$ into $A^{\mathrm{T}}A\boldsymbol{x} =$

$A^T\boldsymbol{b}$, where $A^T$ is the transpose of $A$; after which the standard ICCG algorithm applies.

*Restrictions on the complexity of the problem*
The generator assumes that the nonzero elements of the sparse matrix occur in diagonal bands, as is often the case with finite difference equations. If this pattern does not pertain, then some unnecessary work corresponding to computation on zeros will be produced.

*References*

[1] G. Kuo-Petravic and M. Petravic, Comput. Phys. Commun. 18 (1979) 13.
[2] J.A. Meijerink and H.A. van der Vorst, Math. Comput. 31 (1977) 137.

Computer Physics Communications 22 (1981) 49–58
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# THE VIBRATIONAL EXCITATION OF DIATOMIC MOLECULES BY ELECTRON IMPACT

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Received 15 July 1980

## PROGRAM SUMMARY

*Title of program*: SAS14

*Catalogue number*: AAJF

*Computer*: 370/165; *Installation*: Daresbury Laboratory

*Operating system*: HASP

*Programming language*: FORTRAN IV

*High speed storage required*: 118 Kbytes

*Number of bits in a word*: 64

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 1588

*Keywords*: cross section, vibration, diatomic molecule

*Nature of physical problem*
The scattering of slow electrons by diatomic molecules, producing vibrational excitation.

*Method of solution*
K matrices from the scattering problem are used to obtain differential cross sections.

*Restrictions in the complexity of the problem*
Two open vibrational channels; ten partial waves for each vibrational channel.

*Typical running time*
$1\frac{1}{2}$ s for test data.

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# A FORTRAN SYSTEM TO MAINTAIN A PROGRAM LIBRARY

## 1. Storage of the program decks in magnetic tape files

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Received 19 November 1980

## PROGRAM SUMMARY

*Title of program*: UPDATE

*Catalogue number*: AANE

| *Computer*: | *Installation* |
|---|---|
| (1) ICL 1906S | (1) Queen's University, Belfast |
| (2) IBM 360/195 | (2) Rutherford Laboratory, Chilton, Didcot, Oxfordshire |
| (3) IBM 370/165 | (3) Daresbury Laboratory, Warrington, Cheshire |

*Operating system*: George IV

*Programming language used*: FORTRAN

*High speed store required*: 13248 words

*No. of bits in word*: 24 (ICL 1906S)

*Overlay structure*: none

*No. of magnetic tapes required*: 3 minimum

*Other peripherals used*: card reader, line-printer, disc

*No. of cards in combined program and test deck*: 2712

*Keywords*: information, storage, retrieval, library, file management, character manipulation, general purpose, utility.

*Nature of the physical problem*
This program stores the CPC library of programs serially on magnetic tape files and maintains an index. The card images are contracted in a simple way. It takes as input cards or magnetic tape, in particular a CPC subscriber tape [1], and has the facility to edit existing files.

*Restrictions on the complexity of the problem*
The program is of general use. It can store any library of data in the form of card decks so long as the decks are each serially numbered and identified by a four-character catalogue number.

The editing facility does not include the altering of cards within a deck. It involves the deletion of a deck or the insertion of adaptation or correction decks [2] adjacent to the relevant program.

*Unusual features of the program*
The program involves character manipulation and requires simple subroutines to be supplied by the user to pack and unpack groups of characters into a word. Versions of these routines for the ICL 1906S, IBM 360/195 and the CDC 6600 are included.

There is the facility whereby editing of a multi-reel library is performed as a series of subsidiary runs and therefore the maximum number of tape units required at any one time is three.

*Typical running time*
The central processor time to store 14 programs, approximately 23 700 cards is about 45 s using a subscriber tape as input.

*References*
[1] C. Jackson, Comput. Phys. Commun. 19 (1980) 11.
[2] Instructions to authors, Comput. Phys. Commun. 19 (1980) 1.

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Computer Physics Communications 22 (1981) 77–84
North-Holland Publishing Company

# A FORTRAN SYSTEM TO MAINTAIN A PROGRAM LIBRARY

## 2. Retrieval of program decks from the library files

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Received 19 November 1980

## PROGRAM SUMMARY

*Title of programs*: RETRIEVE, CPSN, CPIN, CREC

*Catalogue numbers*: AANF, AANG, AANH, AANI

| *Computer* | *Installation* |
|---|---|
| (1) ICL 1906S | (1) Queen's University, Belfast |
| (2) IBM 360/195 | (2) Rutherford Laboratory, Chilton, Didcot, Oxfordshire |
| (3) IBM 370/165 | (3) Daresbury Laboratory, Warrington, Cheshire |

*Operating system*: George IV

*Programming language used*: FORTRAN

*High speed storage required*: 8192 words (for RETRIEVE)

*No. of bits in a word*: 24 (ICL 1906S)

*Overlay structure*: none

*No. of magnetic tapes required*: 1

*Other peripherals*: card reader, line printer, card punch, disc

*No. of cards in combined program and test deck*: 1888

*Keywords*: information, storage, retrieval, library, file management, character manipulation, general purpose, utility

*Nature of the physical problem*
Program RETRIEVE retrieves decks, specified by their catalogue numbers from master library files which are copies of the files described in ref. [1]. The files may be serial or direct access. The output medium can be cards or listings. Only one person is supplied in one run. Programs CPSN, CPIN, CREC are auxiliary programs, described in appendices 1 and 2, for file manipulation.

*Restrictions on the complexity of the problem*
The number of catalogue numbers requested is restricted by array lengths which can be altered.

*Unusual features of the program*
Similarly to UPDATE [1], the program involves character manipulation and requires the same packing subroutines described in ref. [1].

*Typical running time*
To retrieve two programs, total length 984 cards, from a magnetic tape program file took 0.03 s mill time. 1950 blocks were read from the tape during the retrieval.

*References*
[1] V.M. Burke and C. Jackson, Comput. Phys. Common. 22 (1981) 59.

Computer Physics Communications 22 (1981) 85–96
North-Holland Publishing Company

# FSCRIPT, A FULL PORTABLE TEXT FORMATTING PROGRAM

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Received 3 October 1980

FSCRIPT is a program designed to handle texts in an easy way. The text is given as card images in an unformatted way together with the desired commands. These commands (there are 33 different commands) control the formatting of the text. FSCRIPT has been written in ANS FORTRAN.

## PROGRAM SUMMARY

*Title of the program*: FSCRIPT

*Catalogue number*: ABVY

*Computer*: IBM 370/155–158; *Installation*: UDAC, Uppsala Datacentral, Sweden

*Operating system*: OS/MVT

*Programming language used*: ANS FORTRAN

*High speed storage required*: 54 kbytes

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: terminal, card reader, line printer

*No. of cards in combined program and test deck*: 1705

*Keywords*: automatic text formatting, full portable program, ANS-FORTRAN

*Nature of the physical problem*
To produce manuscripts, reports and several other types of written documents is a task that the physicist must face far too frequently. FSCRIPT is an automatic formatting program designed to meet these requirements.

*Method of solution*
The text words are read in as card images and the first column of each input card is inspected. If the character "." (period) is found then the input character is considered to have (at least) a command. Otherwise it is taken as a part of the text. If a command is detected then it is analysed and actions are taken according to the values of the operands. Then the input line is further inspected because several commands are allowed in a line. The remainder of the line, after the execution of all the commands, is taken as a part of the input text, unless it is empty. The text words are placed in an array and their positions in it are controlled by the left-margin and the line-length. The array is filled in such a way that no word is split between two lines. Once the line is full the text is right-adjusted (right-justification) and printed out.

*Restriction on the complexity of the problem*
Any type of text may be handled with FSCRIPT. However, the line length must not be less than 15 or greater than 132.

*Typical running time*
The running time depends mainly on the size of the input text and, to a lesser extent, on the number of commands issued. For the test run the CPU-time was 1.42 s on an IBM 370/155–158.

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# J-SQUARE *

Wooil MOON
*Geophysics Division, Department of Earth Sciences, The University of Manitoba,*
*Winnipeg, Canada R3T 2N2*

Received 22 July 1980

## ADAPTATION SUMMARY

*Title of adaptation*: Addition of new function subroutine DJSQ

*Adaptation number*: 0001

*Reference to original program*: ELSGAU

*Catalogue no.*: ACYX

*Author of original program*: Wooil MOON

*Computer*: AMDAHL V7; *Installation*: The University of Manitoba

*Operating system*: OS

*Programming language used*: FORTRAN IV

*High speed storage required*: 44 K

*No. of bits in a word*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards required to effect adaptation*: 53

*Additional keywords*: Geodynamics, *J*-square, coupling

*CPC Library subprograms used*: CF

*Catalogue no.*: ACYK

*Nature of the physical problem*
The *J*-square is a measure of the physical coupling of the normal modes of a vibrating system. The *J*-square appears in the computation of long-period eigenfunctions of realistic Earth models [2]. In the previous study [1], the conventional spherical harmonics are used for normal-mode coupling and one had to evaluate Elsasser and Adams–Gaunt integrals. However, it is found that, in certain cases, the generalized spherical harmonics [3] are much more convenient. The coupling coefficient in this new approach is represented as *J*-square and a numerical scheme to compute *J*-square is included in this adaptation.

*Method of solution*
The *J*-square can be computed using 3-*J* vector coupling coefficient [4] and appropriate selection rules.

*Restrictions on the complexity of the problem*
If each element of *J*-square is clearly defined there is no restriction.

*Typical running time*
0.07 s for test run.

*References*

[1] W. Moon, Comput. Phys. Commun. 16 (1979) 267.
[2] W. Moon, Geophys. J. Roy Astron. Soc. (submitted).
[3] R.A. Phinney and R. Burridge, Geophys. J. Roy. Astron. Soc. 34 (1973) 451.
[4] K. Srinivasa Rao and K. Venkatesh, Comput. Phys. Commun. 15 (1978) 227.

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* The University of Manitoba, Centre for Precambrian Studies, Publication no. 50.

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## ERRATUM NOTICE

*Title of manuscript*: Calculation of LEED diffracted intensities

*Authors*: D.J. Titterington and C.G. Kinniburgh

*Reference*: Comput. Phys. Commun. 20 (1980) 237

*Title of program*: CAVLEED

*Catalogue number*: ABVB

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North-Holland Publishing Company

# RDLIST, A PORTABLE NAMELIST FACILITY

A.C. DAY
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Received 3 October 1980

## PROGRAM SUMMARY

*Title of program*: RDLIST

*Catalogue number*: AANJ

*Computer*: IBM 360/65; *Installation*: University College London, also tested on CDC 6600, CDC 7600, GEC 4082, Cray-1, IBM 370/165, IBM 360/195

*Operating system*: WATFIV for test run

*Programming language used*: FORTRAN IV

*High speed storage required*: 5500 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card-reader, lineprinter

*No. of cards in combined program and test deck*: 425

*CPC Library subprograms used*: *Catalogue number*: AANJ; *Title*: MAKEDATA; *Ref. in CPC*: this paper

*Keywords*: namelist, portable, compatible, character manipulation

*Nature of the physical problem*
Programs often work by setting defaults and requiring users to change only a few of the parameters. The IBM FORTRAN NAMELIST facility is very convenient for this, allowing as it does the use of FORTRAN variable names in the input. The difficulty is that NAMELIST is not generally available. The problem is to write a portable FORTRAN replacement for NAMELIST.

*Method of solution*
The 'NAMELIST' entities are stored in a COMMON block. The names of these entities and any dimensions are stored in a second COMMON block by means of DATA statements in a BLOCK DATA subprogram. These DATA statements are automatically generated from the FORTRAN statement defining the first COMMON block, when this is fed as data into a preprocessor called MAKEDATA. A subroutine RDLIST is provided to read a list of assignments from the input and process them.

*Restrictions on the complexity of the problem*
Only one 'NAMELIST' is permitted. Only REAL variables and arrays are allowed. No repeat counts are possible (e.g. 3 * 1.0 to mean 1.0, 1.0, 1.0). Only input of information is provided for, not output.

*Typical running time*
MAKEDATA takes about 1 s. The time taken by RDLIST depends on the length of the list of input assignments, but typically takes a small fraction of a second per call.

*Unusual features of the program*
Fully portable character manipulation.

*References*

[1] A.C. Day, FORTRAN techniques (Cambridge University Press, London, 1972).
[2] A.C. Day, Compatible FORTRAN (Cambridge University Press, London, 1978).

## PROGRAM SUMMARY

*Title of program*: MAKEDATA

*Catalogue number*: AANJ

*Computer*: IBM 360/65; *Installation*: University College London, also tested on CDC 6600, CDC 7600, GEC 4082, Cray-1, IBM 370/165, IBM 360/195

*Operating system*: WATFIV for test

*Progtamming language used*: FORTRAN IV

*High speed storage required*: 4500 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card-reader, lineprinter, cardpunch

*No. of cards in combined program and test deck*: 312

*Keywords*: namelist, portable, compatible, character manipulation

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North-Holland Publishing Company

# AIRY FUNCTION WITH COMPLEX ARGUMENTS *

Wooil MOON
*Geophysics Division, Department of Earth Sciences, The University of Manitoba, Winnipeg, Canada R3T 2N2*

Received 5 September 1980

## PROGRAM SUMMARY

*Title of program*: AIRY

*Catalogue number*: ABVX

*Computer*: AMDAHL V7; *Installation*: The University of Manitoba Computing Centre

*Operating system*: OS

*Programming language used*: FORTRAN IV

*High speed storage required*: 18 K

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 443

*Key words*: Airy function

*Nature of the physical problem*
In theoretical seismology and electromagnetic theory, the Airy function often appears as a part of solutions and its usefulness can never be exaggerated in applied mathematics in general. This subroutine is written with particular applications in mind to be used in problems where the arguments become complex quantities.

*Method of solution*
For $|z| < 3.5$, the ascending series formulae are used and for $|z|$ greater than 3.5, the asymptotic formulae. These formulae are given by Abramowitz and Stegun [1]. The critical number 3.5 is set arbitrarily in this case, and it can be changed to a more appropriate number as may be necessary. The accuracy of the Airy functions $\mathrm{Ai}(z)$, $\mathrm{Bi}(z)$ and their derivatives is set by the remainder term of the $\mathrm{Ai}(z)$ series which is set to be less than 1.0D–6. If this is found to be inappropriate for $\mathrm{Bi}(z)$ or the derivatives the error criteria can be changed easily in the program. However, the accuracy of the solution will not improve in the vicinity of $|z| = 3.5$, due to the inherent nature of the asymptotic series and ascending series.

*Restrictions on the complexity of the problem*
There are no restrictions as long as the formulae are valid.

*Typical running time*
2.71 s CPU.

*References*

[1] M. Abramowitz and I.A. Stegun, Handbook of mathematical functions (Dover, New York, 1970) p. 446.

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* The University of Manitoba, Center for Precambrian Studies Contribution no. 51.

Computer Physics Communications 22 (1981) 419–432
North-Holland Publishing Company

# A PROGRAM FOR FITTING AND PLOTTING AMPLITUDES, POLARIZATION AND DIFFERENTIAL CROSS SECTION DATA FOR TWO-BODY REACTIONS *

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and

P. KOEHLER
*Stanford Linear Acceleration Center, Stanford University, Stanford, CA 94305, USA*

## PROGRAM SUMMARY

*Title of program*: EXCAMP

*Catalogue number*: ABVW

*Computer*: CDC 6600; *Installation*: University of London Computer Centre

*Operating system*: NOS/BE

*Programming language used*: FORTRAN IV

*High speed store required*: 53 Kwords (includes MINUITS (10 K) and APLOT and other plot controlling routines (16 K))

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, CalComp (or CalComp-compatible) plotter or microfilm plotter

*Number of cards in combined program and test deck*: 3980

*CPC library subprograms used*: MINUITS (ref. in CPC: 10 (1975) 343); APLOT (ref. in CPC: 9 (1975) 85, 15 (1978) 437)

*Keywords*: nuclear, high energy, s-channel helicity amplitudes, amplitude analysis, polarization, Wolfenstein parameters, differential cross section, Gribov–Reggeon calculus, $\chi^2$ minimization

*Nature of the physical problem*
This program is concerned with the phenomenological analysis of high-energy $0^-\frac{1}{2}^+ \to 0^-\frac{1}{2}^+$ scattering processes in terms of $\chi^2$ fits to amplitude, polarization and differential cross section data. Although the program is written for a model of the amplitudes using the Gribov–Reggeon calculus [1] it can be readily adapted by the user to all other models.

*Method of solution*
Amplitude analysis has become an important tool in obtaining phenomenological models for high-energy scattering. Procedures, such as that given in ref. [2], which only fit differential cross sections, do not give enough control on all the features of the model used.

The amplitudes were fitted using the scheme of Halzen and Michael [3] where the isovector amplitudes are defined relative to the isoscalar nonflip amplitude. The program could, however, be readily adapted to produce fits to the real and imaginary parts of the amplitudes (e.g. the pion–nucleon amplitude analysis of Höhler et al. [4]). The program is designed to be used under control of the MINUITS minimization package [5]; a considerable amount of core can be saved when no fitting is required, if MINUITS is replaced by a routine to read in the MINUITS parameters. Plotting of amplitudes, polarization and differential cross sections is achieved using APLOT [6] and the WORDS routine (together with associated routines) [7], the latter for producing the

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* Work supported by the Department of Energy, contract DE-AC03-76SF00515.

special lettering used. Again the program is designed so that when no plotting is required (e.g. when fitting) the plotting packages can be omitted with core saved.

*Restrictions on the complexity of the program*
To save computing time, since the program was only used for $\pi^-p \rightarrow \pi^0n$ with amplitude fitting only at 6 GeV/*c*, the phase prescription due to Ambats et al. [8] for the isoscalar amplitude was used to produce the required parallel and perpendicular components of the amplitudes. This restriction can easily be removed; the user could calculate his own isoscalar amplitudes and use them to produce the required isovector amplitude components. Certain other restrictions on the number of processes, number of energy sets, number of data sets and number of experimental points, are described in the comment section of the routine FCN; these are connected with the dimensions of arrays used and can be reset by the user.

*Typical running time*
The test run (no minimization) took 60 s of which 17 s was compilation time. On a minimization run, when the program was operating at its most efficient rate, the time taken per call to the routine FCN (for total $\chi^2$ calculation) was about 0.22 s.

*References*

[1] R.W.B. Ardill, P. Koehler and K.J.M. Moriarty, SLAC-PUB-2452 (January 1980).
R.W.B. Ardill, K.J.M. Moriarty and P. Koehler, SLAC-PUB-2467 (February 1980).
[2] P.A. Collins, B.J. Hartley, R.W. Moore and K.J.M. Moriarty, Comput. Phys. Commun. 5 (1973) 349.
[3] F. Halzen and C. Michael, Phys. Lett. 36B (1971) 367.
[4] G. Höhler, F. Kaiser, R. Koch and E. Pietarinen, Physik Daten/Physics Data. Handbook of pion–nucleon scattering, Institut für Theoretische Kernphysik der Universität Karlsruhe, Fed. Rep. Germany (1979).
[5] F. James and M. Roos, Comput. Phys. Commun. 10 (1975) 343.
[6] J. Anderson, K.J.M. Moriarty and R.C. Beckwith, Comput. Phys. Commun. 9 (1975) 85.
J. Anderson, R.C. Beckwith, K.J.M. Moriarty and J.H. Tabor, Comput. Phys. Commun. 15 (1978) 437.
[7] Imperial College London program library ICMICFILMFTN.
[8] I. Ambats et al., Phys. Rev. D9 (1974) 1179.

Computer Physics Communications 22 (1981) 433–437
North-Holland Publishing Company

# MONTE CARLO SIMULATION OF U(1) LATTICE GAUGE THEORY

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*Department of Mathematics, Royal Holloway College, Egham, Surrey TW20 0EX, UK*

and

K.J.M. MORIARTY *
*DESY, Hamburg, Fed. Rep. Germany*

Received 18 November 1980

## PROGRAM SUMMARY

*Title of program*: U1LATTICE

*Catalogue number*: ABEA

*Computer*: CDC 7600; *Installation*: ULCC

*Operating system*: SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: 16 Kwords

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Total no. of cards in combined program and test deck*: 430

*Keywords*: lattice gauge theory, U(1), quark confinement, phase diagram, phase transition, statistical mechanics, action per plaquette, Monte Carlo

*Nature of the physical problem*
The program calculates the average action per plaquette for U(1) lattice gauge theory. Gauge theories formulated on a lattice were proposed by Wilson [1] and Polyakov [2], and the average plaquette action is an important observable in the study of phase transitions in such systems.

*Method of solution*
A Monte Carlo simulation of the lattice system, using the heat bath method of ref. [3] adapted to U(1), generates a series of field configurations approximating statistical equilibrium at a given temperature.

*Restrictions on the complexity of the program*
The storage required is dependent on the lattice size. The execution time increases with the lattice size and with the number of Monte Carlo iterations required, and is typically rather long. At temperatures much below the critical point the Monte Carlo vetoing process becomes very slow.

*Typical running time*
The test run took 34 s on the CDC 7600 at ULCC.

*References*

[1] K.G. Wilson, Phys. Rev. D10 (1974) 2455.
[2] A.M. Polyakov, unpublished.
[3] M. Creutz, L. Jacobs and C. Rebbi, Phys. Rev. D20 (1979) 1915.

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Computer Physics Communications 22 (1981) 439–450
North-Holland Publishing Company

# A PROGRAM TO SOLVE A SOLUTE DIFFUSION PROBLEM WITH SEGREGATION AT A MOVING INTERFACE

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and

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Received 19 December 1980

## PROGRAM SUMMARY

*Title of program*: DIFSEG

*Catalogue number*: ABVZ

*Installation*: SARA (Academic Computing Centre Amsterdam)

*Plotting library used*: CALCOMP, available at SARA

*Operating system*: NOS/BE

*Programming language*: FORTRAN IV

*High speed storage requested*: 128 K

*No. of bits in a word*: 60

*Overlay structure*: none

*Other peripherals used*: card reader, line printer, plotter and scratch disk store (the last one only if the plotter is used)

*No of cards in combined program and test deck*: 911

*Key words*: silicon, laser-annealing, solute-segregation, diffusion equation, finite difference method, moving boundary problem

*Nature of the physical problem*
The diffusion and segregation of impurities implanted in silicon which accompany the annealing of implantation damage by means of pulsed-laser irradiation.

*Method of solution*
The diffusion equation is semidiscretized by the finite difference method and the resulting ODE is integrated by an adapted Runge–Kutta method.

*Running time*
Roughly proportional to the dimension of the ODE.

*Unusual features*
The user should have no difficulty in replacing the CALCOMP plotting routines by equivalent routines at his own installation, using figs. 4–7 as examples.

Computer Physics Communications 22 (1981) 451–466
North-Holland Publishing Company

# THE CODE FRANPIE: A SEMICLASSICAL FRICTION FREE MODEL FOR CALCULATING EXCITATION FUNCTIONS FOR COMPLETE FUSION OF HEAVY IONS *

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Received 1 October 1980

## PROGRAM SUMMARY

*Title of program*: FRANPIE

*Catalogue number*: ABPK

*Computer*: IBM 360, IBM 370, B6700 and UNIVAC 1100; *Installation*: Computing Center, State University of New York at Stony Brook, Stony Brook, NY 11794, USA

*Operating system*: UNIVAC 1100 Time/Sharing Exec – Multiprocessor System

*Programming language used*: Fortran

*High speed storage required*: 20180 words

*Number of bits in a word*: 36

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 1345

*Keywords*: nuclear, semiclassical friction free model, real potential, complete fusion, fusion barrier, critical angular momenta, critical radii

*Nature of the physical problem*
The complete fusion cross section is calculated as a function of energy with a semiclassical friction free model. No allowance is made (1) for energy and angular momentum dissipation due to particle emission (e.g. $^4$He/$^1$H) prior to fusion, and (2) for loss of low partial waves due to highly inelastic events. The cross section is calculated by partial wave summation. Barrier penetration is included and so is the $l$ dependence of the fusion radius and the curvature of the barrier.

*Method of solution*
The real potential may take a number of forms. Provision is made to alter parameter of nuclear and Coulomb potentials so that a best match to the experimental fusion barrier/cross sections can be achieved.

*Restrictions on the complexity of the problem*
Calculations are straightforward and involve no complexity.

*Typical running time*
Typical running time (CPU) on the UNIVAC 1100 is 2.475 s for tabulated form of the nuclear proximity function and slightly over 0.3 s for the other options and/or combination of options. Typical I/O time is about 1.7 s.

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Computer Physics Communications 22 (1981) 467–472
North-Holland Publishing Company

# *R*-MATRIX DYNAMIC DIPOLE POLARIZABILITIES

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Received 21 July 1980; in revised form 15 December 1980

## ADAPTATION SUMMARY

*Title of adaptation*: *R*-Matrix Polarizabilities

*Adaptation number*: 0001

*Reference to original program*
*Cat. No.*: AAHH;
*Title*: A New Version of RMATRX STG3;
*Ref. in CPC*: 14 (1978) 367–412

*Authors of original program*: K.A. Berrington, P.G. Burke, M. LeDourneuf, W.D. Robb, K.T. Taylor and Vo Ky Lan

*Computer*: IBM 370/165; *Installation*: Science Research Council, Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England

*No. of bits in a word*: 32

*No. of cards required to effect adaptation (including directive cards)*: 428

*CPC Library subprograms used*:

| *Catalogue no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAHF | A NEW VERSION OF RMATRX STG1 | 14 (1978) 367 |
| AAHG | A NEW VERSION OF RMATRX STG2 | 14 (1978) 367 |
| AAHH | A NEW VERSION OF RMATRX STG3 | 14 (1978) 367 |

*Additional keywords*: *R*-matrix, dynamic polarizabilities

*Nature of the physical problem*
The lowest order interaction of electromagnetic radiation with an atom is directly related to the frequency dependent multipole polarizability. A knowledge of the dynamic polarizability of the system is therefore important in determining level shifts, refractive indices, harmonic coefficients, the Van der Waals $C_6$ coefficient and similar quantities relating to the response of an atom to a perturbing field. The dynamic dipole polarizability can be written in several forms, length and velocity being two of the most common. In the length form, the tensor polarizability is given by

$$\alpha^{l}_{M_L M'_L \mu\nu}(\omega) = 2\sum_i (E_i - E_0) \times \langle\Phi_0(LM'_L)|M^{\mu}_{1l}|\Phi_i(L_iM_{L_i})\rangle \times \langle\Phi_i(L_iM_{L_i})|M^{\nu}_{1l}|\Phi_0(LM_L)\rangle/[(E_i - E_0)^2 - \omega^2] \qquad (1)$$

or alternatively by

$$\alpha^{l}_{M_L M'_L \mu\nu}(\omega) = \sum_i \langle\Phi_0|M^{\mu}_{1l}|\Phi_i\rangle\langle\Phi_i|M^{\nu}_{1l}|\Phi_0\rangle \times\left[\frac{1}{E_i - E_0 + \omega} + \frac{1}{E_i - E_0 - \omega}\right], \qquad (2)$$

where $M^{\mu}_{1l}$ is the $\mu$th standard tensor component of the position operator, with similar expressions involving the other forms of the matrix element. The polarizability thus can be determined by explicitly performing the summation over intermediate states. This procedure, however, can often be unsatisfactory because of the prohibitively large number of terms which may need to be retained in the summation in order to produce useful results. Alternative procedures to the explicit summation method are therefore required.

*Method of solution*
Using the method of Dalgarno and Lewis [1] the summations over intermediate states are first replaced by differential equations. These differential equations are then solved using

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straightforward atomic $R$-matrix methods [2,3]. The method is readily implemented by making the observation that the non-homogeneous term in each of the equations vanishes for radial distances greater than the $R$-matrix radius.

*Restrictions on the complexity of the problem*
Same as for standard RMATRX.

*Typical running time*
Neon test case using data as for standard RMATRX STG3 – approx. 40 photon energies per 20 s, without the Buttle correction.

*References*

[1] A. Dalgarno and J.T. Lewis, Proc. R. Soc. London Ser. A233 (1955) 70.
[2] P.G. Burke, A. Hibbert and W.D. Robb, J. Phys. B4 (1975) 153.
[3] P.G. Burke and W.D. Robb, in: Advances in atomic and molecular physics, vol. 11, eds. D.R. Bates and B. Bederson (Academic Press, London, 1975).

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Computer Physics Communications 23 (1981) 31–42
North-Holland Publishing Company

# HFATER: A 2D LASER PROPAGATION SUBROUTINE FOR UNDERDENSE PLASMAS

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Received 5 January 1981

## PROGRAM SUMMARY

*Title of program*: HEATER

*Catalogue number*: ABSG

*Computer*: Amdahl 470/V7; *Installation*: Univ. of Alberta

*Operating system*: Michigan Terminal System

*Programming language used*: Fortran IV

*High speed store required*: 36934 bytes

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 601

*Keywords*: laser propagation, laser heating, refraction, diffraction, absorption, cubic spline

*Nature of the physical problem*
The physical problem is to describe the propagation of a laser beam in a cylindrically symmetric, underdense plasma given the electron density, electron temperature, ionization number and characteristics of the incoming beam. The solution is to be calculated in a subroutine which can be used with 2D simulation codes such as CASTOR 2 [1].

*Method of solution*
The subroutine defines its own 2D mesh based on the mesh of the main simulation code and uses a cubic spline technique [2] to solve the propagation equation for the laser.

*Restrictions on the complexity of the problem*
Cylindrical symmetry is assumed for the plasma and the beam, and the incoming beam is assumed to have a Gaussian cross-section. The approximations used to derive the propagation equation break down when the density is close to the critical density. Anomalous effects are not included.

*Typical running time*
If the internal mesh is calculated, one call to the subroutine requires approximately 0.7 s on the Amdahl 470/V7 (approximately equivalent to the IBM 3033). Approximately 0.6 s are required if the mesh has been calculated in a previous call. These times will increase if the internal mesh is made finer in an attempt to gain more accuracy but do not depend on the coarseness of the external mesh of the calling program.

*References*

[1] J.P. Christiansen and N.K. Winsor, Comput. Phys. Commun. 17 (1979) 397.
[2] J.A. Fleck, Jr., J. Comput. Phys. 16 (1974) 324.

Computer Physics Communications 23 (1981) 43–50
North-Holland Publishing Company

# A PROGRAM FOR CALCULATING THE STRUCTURE FACTORS OF LIQUID METALS AND BINARY LIQUID ALLOYS

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Received 22 September 1980

## PROGRAM SUMMARY

*Title of program:* AVA

*Catalogue number:* ACKT

*Computer:* CDC 7600; *Installation:* University of London Computer Centre

*Operating system:* SCOPE 2.1.5

*Programming language used:* FORTRAN IV

*High speed store required:* 3064 words

*Number of bits in a word:* 60

*Is the program overlaid:* no

*Other peripherals used:* card reader, line printer

*Number of cards in combined program and test deck*: 310

*Keywords:* liquid metal, binary liquid alloy, structure factor, resistivity, thermopower, packing-fraction, hard-sphere

*Nature of the physical problem*
This program computes the structure factor of liquid metals and binary liquid alloys.

*Method of solution*
The formulae, based on the Percus–Yevick hard sphere model, for the structure factor given by Ashcroft and Lekner [1] for liquid metals and by Ashcroft and Langreth [2] for binary liquid alloys are used.

*Restriction on complexity of the problem*
The starting value of Y (see section 3) which is fixed to Y = 0.25 in the program may be altered if necessary. However, Y = 0.0 should not be assigned in order to avoid the problem of overflow.

*Typical running time*
Compilation time: 0.23 s, execution time of sample data: 0.03 s.

*References*
[1] N.W. Ashcroft and J. Lekner, Phys. Rev. 145 (1966) 83.
[2] N.W. Ashcroft and D.C. Langreth, Phys. Rev. 156 (1967) 685.

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Computer Physics Communications 23 (1981) 51–61
North-Holland Publishing Company

# A PROGRAM FOR COMPUTING THE CONICAL FUNCTIONS OF THE FIRST KIND $P^m_{-1/2+i\tau}(x)$ FOR $m = 0$ AND $m = 1$

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Received 28 November 1980

## PROGRAM SUMMARY

*Title of program*: FCONIC

*Catalogue number*: AAQH

*Computer*: CDC 7600; *Installation*: CERN, Geneva

*Operating system*: CDC scope

*Programming language used*: FORTRAN IV

*High speed store required*: 1164 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 853

*Keywords*: conical function, Legendre function, spherical functions, boundary value problems, integral transforms, Mehler–Fock transform, asymptotic expansions

*Nature of the physical problem*
The conical functions $P^m_{-1/2+i\tau}(x)$ appear in a wide range of physical applications. Here we mention boundary value problems for the Laplace equation in regions bounded by cones, by two intersecting spheres, or by one or two confocal hyperboloids of revolution. Further, these functions are used in the Mehler–Fock integral transform for problems in potential and heat theory, and in elementary particle physics.

*Method of solution*
Series expansions based on Gaussian hypergeometric functions evaluated by direct summation or rational approximations are used together with asymptotic expansions for real $x > -1$ and real $\tau \geqslant 0$.

*Accuracy*
As the tests show, an accuracy of at least approximately 10 significant digits is normally obtained. The $x$ and $\tau$ not too large, the accuracy increases to about 12–13 significant digits.

*Running time*
A running time of about 300 μs on a CDC 7600 was found o the average. For $x > 0$ and $\tau > 20$, the time reduces to about 200 μs on the average.

Computer Physics Communications 23 (1981) 63–80
North-Holland Publishing Company

# ATHENE 1A: A ONE-DIMENSIONAL FUSION CODE

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Received 27 February 1981

## PROGRAM SUMMARY

*Title of program*: ATHENE 1A

*Catalogue number*: ABQI

*Computer*: ICL 2976; *Installation*: UKAEA Culham Laboratory. The program can be used on any computer equipped with the OLYMPUS system

*Operating system*: ICL VME/B

*Programming language used*: FORTRAN

*High speed store required*: 197 000 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 12 570

*CPC Library subprograms used*:

| *Catalogue no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ABUF | OLYMPUS (ICL 4/70) | 7 (1974) 245 |
| ABUJ | OLYMPUS (IBM 370/165) | 9 (1975) 51 |
| ABUK | OLYMPUS (CDC 6500) | 10 (1975) 167 |

Alternative versions already published.

*Keywords*: plasma physics, thermonuclear fusion, pinch devices, reversed field pinches, one-dimensional equilibrium, diffusion, implicit, impurities, impurity transport, ionisation

*Nature of the physical problem*
The purpose of ATHENE 1A is to calculate the evolution of a high-$\beta$ toroidal CTR plasma in the cylindrical approximation, taking into account diffusion and other entropy-generating processes in a plasma which evolves through a sequence of magnetohydrodynamic pressure equilibria. The ATHENE 1A model is an extension of the previously published code ATHENE 1 [1].

*Method of solution*
The plasma and the magnetic field are described by five main variables and up to 5 impurity concentration levels which are functions of the time $t$ and a single radial space variable $r$. The solution of the MHD equations in these ten variables is split into two stages. In stage 1, which uses a fixed Eulerian mesh, diffusion and other processes change the entropy of the plasma-field configuration. Stage II is a Lagrangian calculation.

*Restrictions on the complexity of the problem*
Version 1 of ATHENE 1A provides a simple model for the behaviour of plasma-pinch configurations. A number of physical effects such as ionization, recombination and diffusion of plasma impurities have been added and additional physics can easily be included in the code, e.g., by use of the EXPERT facility [2,3]. In ATHENE 1A the initial radial profiles of the main variables can be altered as required and the operation of the code follows that outlined in ref. [1].

### *Unusual features of the program*

ATHENE 1A is written in OLYMPUS FORTRAN, i.e. standard FORTRAN [4] except for the use of the NAMELIST facility. The structure of the code is based on the OLYMPUS system [2,3] in order to facilitate transfer to other types of computer.

### *References*

[1] J.P. Christiansen, K.V. Roberts and J.W. Long, Comput. Phys. Commun. 14 (1978) 423.

[2] K.V. Roberts, Comput. Phys. Commun. 7 (1974) 237.

[3] J.P. Christiansen and K.V. Roberts, Comput. Phys. Commun. 7 (1974) 245.

[4] Standard Fortran Programming Manual, Computer Standards Series, National Computing Centre Ltd., Manchester England (1970).

Computer Physics Communications 23 (1981) 81–93
North-Holland Publishing Company

# COMPUTATION OF GROUP TABLES FOR THE SYMMETRIC GROUPS

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Received 24 September 1980; in revised form 26 November 1980

## PROGRAM SUMMARY

*Title of program*: SYMGRPTB

*Catalogue number*: AAMC

*Computer*: IBM 3033; *Installation*: City University of New York – University Computer Center

*Operating system*: OS/MVT/ASP

*Programming language used*: PL/I Optimizer

*High speed storage required*: 228 kbytes through S(4)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required (if used)*: 1

*Other peripherals used*: card reader, line printer, card punch or tapes

*No. of cards in combined program and test deck*: 746

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAME | SYMSTATS | 23 (1981) 95 |

*Keywords*: general purpose, symmetric group, group generators, permutations, group multiplication table, explicit construction

*Nature of the physical problem*
To find explicitly the generators (permutations) and group multiplication tables for the symmetric groups.

*Method of solution*
The permutations of S(NMAX) are found by inserting parentheses, at positions determined by the computed row lengths of the frames, into the NMAX! strings of permutations of the numerals 1 ... NMAX. The group table is found by multiplying every pair of permutations, and searching for the permutation which is the same as their product.

*Restrictions of the size of the problem*
The program can be used for any symmetric group, for which machine time and storage are available. However, for S(10) and above, there must be some modifications because the numbers then consist of two digits.

*Typical running times*
Through S(4): 20.71 s.

## PROGRAM SUMMARY

*Title of program*: NGHBTRNS

*Catalogue number*: AAMD

*Computer*: IBM 3033; *Installation*: City University of New York – University Computer Center

*Operating system*: OS/MVT/ASP

*Programming language used*: PL/I Optimizer

*High speed storage required*: 194 kbytes through S(4)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required (if used)*: 1

*Other peripherals used*: card reader, line printer, card punch or tapes

*No. of cards in combined program and test deck*: 132

*Card punching code*: EBCDIC

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAME | SYMSTATS | 23 (1981) 95 |
| AAMC | SYMGRPTB | this paper |

*Keywords*: general purpose, symmetric group, permutations, neighboring transpositions, explicit decompositions

*Nature of the physical problem*

To find the set of neighboring transpositions which is equivalent to each permutation of any symmetric group.

*Method of solution*

The decomposition follows immediately from the theorem [1] proving the decomposition's existence. The programming is a direct restatement of this result. The outside of the main program is similar to that of SYMGRPTB. The subroutine packages used are ROWLEN, GENPERM and FAC. It is in the subroutine NR of GENPERM that the decomposition is actually found. The main program, inside a DO-loop on the permutations calls the subroutine NR to find the decomposition for the permutation given by the loop index. Once found, it is written out on tape, in the matrix TS (indexed by the permutation and by the transposition index).

The decomposition is done twice, once when the permutations are constructed, and again in this loop, before the result is actually stored on tape. This could have been avoided by inserting the matrix TS into GENPERM. But this would have introduced an unnecessary matrix into the other programs using this subroutine. It was felt better to have the inefficiency here than in the more important programs.

The maximum number of neighboring transpositions into which a permutation may be decomposed, for each symmetric group, is needed to set the bounds on the relevant matrices. The formula for it was found previously [2], and appears here as the variable MNT, calculated at the beginning of the program from the formula (actually 1 greater than given by the formula, to avoid problems when bounds of DO-loops are being checked).

*Program checks*

The decomposition subroutine is used in several paths of the other programs of this set, so its correctness is checked in checking them. That the transpositions are output properly can be checked by seeing that every permutation (except the identity) is decomposed, that the number of transpositions does not exceed the value given by the formula (the bounds are set so it can, by 1), that the neighboring transpositions are correctly decomposed into themselves, and by spot checking by hand.

The output is NF, then each NMAX followed by the decomposition of each permutation, in the form of the matrix TS, which is also output on tape.

*Restrictions of the size of the problem*

The program can be used for any symmetric group, for which machine time and storage are available. However, for S(10) and above, there must be some modifications because the numbers then consist of two digits.

*Typical running times*

Through S(4): 12.09 s.

*References*

[1] D.E. Rutherford, Substitutional analysis (Cambridge Univ. Press, Cambridge, 1948) p. 5.
[2] M. Soto and R. Mirman, J. Math. Phys. (to be published).

Computer Physics Communications 23 (1981) 95–107
North-Holland Publishing Company

# CONSTRUCTION OF SYMMETRIC GROUP REPRESENTATION MATRICES AND STATES

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Received 24 September 1980; in revised form 26 November 1980

## PROGRAM SUMMARY

*Title of program*: SYMSTATS

*Catalogue number*: AAME

*Computer*: IBM 3033; *Installation*: City University of New York – University Computer Center

*Operating system*: OS/MVT/ASP

*Programming language used*: PL/I Optimizer

*High speed storage required*: 216 kbytes through S(4)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required (if used)*: 1

*Other peripherals used*: card reader, line printer, card punch or tapes

*No. of cards in combined program and test deck*: 769

*CPC library subptograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAMC | SYMGRPTB | 23 (1981) 81 |

*Keywords*: general purpose, symmetric group, irreducible representation, representation matrices, basis vectors, basis states, basis state operators, explicit construction

*Nature of the physical problem*
To find explicitly basis states and basis state operators for the symmetric groups, in a form applicable to any symmetric group and most useful for applications.

*Method of solution*
The states are realized by sums of products of boson-type operators, whose indices show the permutations, concatenated with the relevant matrix elements. They are produced by direct construction.

*Restrictions on the size of the problem*
The program can be used for any symmetric group, for which machine time and storage are available. However, for S(10) and above, there must be some modifications because the numbers then consist of two digits.

*Typical running times*
Through S(4): 30.00 s.

## PROGRAM SUMMARY

*Title of program*: SYMRPMAT

*Catalogue number*: AAMF

*Computer*: IBM 3033; *Installation*: City University of New York – University Computer Center

*Operating system*: OS/MVT/ASP

*Programming language used*: PL/I Optimizer

*High speed storage required*: 174 kbytes through S(4)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required (if used)*: 1

*Other peripherals used*: card reader, line printer, card punch or tapes

*No. of cards in combined program and test deck*: 171

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAMC | SYMGRPTB | 23 (1981) 81 |
| AAME | SYMSTATS | this paper |

*Keywords*: general purpose, symmetric group, representation matrix, permutation, explicit numerical values

*Nature of the physical problem*
To find the explicit representation matrices for every permutation, for every representation, for any symmetric group.

*Method of solution*
The representation matrices for the neighboring transpositions are found from the formulas [1]. Every permutation can be written as a product of neighboring transpositions [2]. Thus, the representation matrix for a permutation is found by simply multiplying the matrices of the neighboring transpositions into which the permutation decomposes.

The main program is similar to SYMSTATS, in setting variables and calling the subroutines which are standard to all the programs in this set. The subroutine packages used are ROWLEN, GENPERM, FAC and CONSMAT. It is in the subroutine RM of the latter package that the matrices are actually found.

In the main program there are DO-loops over the representations, and over the permutations, inside of which is a call to RM to compute the matrix for the current permutation. It is stored in UTR, indexed by the permutation index and by the matrix row and column indices.

There are two structures found in the program, in order to provide a convenient way of placing on tape parameters needed by the programs which reformat and check (and in other ways may use) the matrices. One is NUMTRNS, which contains the variable LH, the largest dimension of any of the representations of the current symmetric group (plus 1 to avoid problems when DO-loop bounds are checked), and NRP, the estimate of the number of representations of the current group. The other is DATTRNS, which contains IG, the set of dimensions and NU, the number of dimensions for each symmetric group up to, and including, the present one. The variables in the structures all end in T, and are used to transfer the corresponding variables to the other programs (the variables themselves could not be in the structures since these are DECLAREd inside the DO-loop giving the symmetric group, and thus would be reinitialized).

The output of the program is NF, which gives the largest symmetric group considered, then for each NMAX, the value of NMAX and the two structures, followed for each representation by NMAX and KA, the representation index, and then by the matrices, UTR, for that representation.

The results of this program are checked by the accompanying program MATTAB. That it is running correctly can be seen by checking that all representations for each NMAX are printed out, for all permutations, and that the neighboring transpositions are correct.

*Restrictions of the size of the problem*
The program can be used for any symmetric group, for which machine time and storage are available. However, for S(10) and above, there must be some modifications because the numbers then consist of two digits.

*Typical running times*
Through S(4): 23.18 s.

*References*

[1] S. Schindler and R. Mirman, J. Math. Phys. 18 (1977) 1678.
[2] D.E. Rutherford, Substitutional analysis (Cambridge Univ. Press, Cambridge, 1948) p. 5.

## PROGRAM SUMMARY

*Title of program*: ORTHNRM

*Catalogue number*: AAMG

*Program obtainable from*: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

*Computer*: IBM 3033; *Installation*: City University of New York – University Computer Center

*Operating system*: OS/MVT/ASP

*Programming language used*: PL/I Optimizer

*High speed storage required*: 224 kbytes through S(4)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required (if used)*: 1

*Other peripherals used*: card reader, line printer, card punch or tapes

*No. of cards in combined program and test deck*: 200

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAME | SYMSTATS | this paper |

*Keywords*: symmetric groups, basis states, orthonormality, verification

*Nature of the physical problem*
To check that the states produced by SYMSTATS form an orthonormal set.

*Method of solution*
An acceptable basis for the representations of the symmetric group consists of a set of multinomials, over which the action of the generators of the group is defined, which are complete and orthonormal. Orthonormality requires the definition of the product of terms. We define the product of any single product of boson terms with any other single product of terms as 1 if all the indices are in the same order in both terms, zero otherwise. From this the product of sums can be found.

This program verifies that the computed states are orthonormal. For each value of NMAX, the product of every state of every representation with every state of every representation is found. This product should be zero, except when the two states are identical, when it should be 1.

In both states of a product, the terms corresponding to the different permutations are in the same order. Thus to find the product, what is done is to take the product of each of the two coefficients of each of the corresponding terms and sum them. Then the result is divided by the product of the normalization coefficients. These coefficients are given by the vector TH.

The output, after NF, is the value of NMAX, with the normalization coefficients, the TH matrix, then followed, for each pair of states by the indices then the product, which is PS. This should be 1 if the first two indices are the same, the third and fourth are the same, and the fifth and sixth are also the same, zero otherwise. After PS, on the same line, is PSC, which is the correct value. These two numbers should agree (within rounding errors). One disagreement indicates an error. If there is a disagreement, the program outputs 4 blank lines (for emphasis) then "ERROR".

*Restrictions of the size of the problem*
Any data produced by SYMSTATS can be checked. However, for S(10) and above, there must be some modifications because the numbers then consist of two digits.

*Typical running times*
Through S(4): 16.78 s.

## PROGRAM SUMMARY

*Title of program*: MATTAB

*Catalogue number*: AAMH

*Computer*: IBM 3033; *Installation*: City University of New York University Computer Center

*Operating system*: OS/MVT/ASP

*Programming language used*: PL/I Optimizer

*High speed storage required*: 222 kbytes through S(4)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required (if used)*: 1

*Other peripherals used*: card reader, line printer, card punch or tapes

*No. of cards in combined program and test deck*: 214

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAMC | SYMGRPTB | 23 (1981) 81 |
| AAME | SYMSTATS | this paper |
| AAMF | SYMRPMAT | this paper |

*Keywords*: symmetric groups, group tables, representation matrices, matrix product, verification

*Nature of physical problem*
To check that the representation matrices produced by SYMRPMAT satisfy the group table produced by SYMGRPTB.

*Method of solution*
The programs in this set have been checked for the situations in which they have been run. However, it is always possible that for some S(N), different for the values for which the checks were made, a bug will appear. This most likely could occur because the sizes of the objects depends on N. Moreover, it is also possible that in a different environment than that in which they were developed, different computer, different operating system, different implementation of the language, etc., they may behave somewhat differently, and possible incorrectly. Thus, it is useful to check the output. For this reason two check programs are included here.

The representation matrices are defined to satisfy the product law given by the group table. Any set of matrices which satisfies this law forms a representation. Of course, it need not be either faithful or irreducible, but these do not raise relevant problems here.

This program checks that the computed matrices satisfy the group table found for each symmetric group. At the same time it thereby checks that the group table is correct. The program is also useful in giving estimates of the precision of the matrix elements.

For each representation the product of every pair of matrices is found, and denoted by U1. From the group table the product of the corresponding permutations is known, and stored in the matrix NPERMS, indexed by the indices of the two permutations. So the corresponding matrix for the product permutation is known. The matrix UD which is the difference between this and U1 is then calculated.

This matrix should be exactly zero. However, because of rounding errors it will not be exactly so. The program is instructed to flag an error, and list the term ERROR if any one of the matrix elements is greater than (the arbitrarily chosen value of) CTF = $10^{-2}$. With the term ERROR it also lists the incorrect matrix element indices, the indices of the two permutations and the difference matrix. After checking a matrix it lists CORRECT (whether the matrix was or not), the indices of the permutations and the difference matrix.

*Restrictions on the size of the problem*
Any data produced by SYMGRPTB and SYMRPMAT can be checked. However, for S(10) and above, there must be some modifications because the numbers then consist of two digits

*Typical running times*
Through S(4): 14.25 s.

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## ERRATUM NOTICE

*Title of manuscript*: CASTOR 2, a two-dimensional laser target code
*Authors*: J.P. Christiansen and N.K. Winsor
*Reference*: Comput. Phys. Commun. 17 (1979) 397
*Title of program*: CASTOR 2
*Catalogue number*: ABUY

Computer Physics Communications 23 (1981) 135–143
North-Holland Publishing Company

# A SPLINE FUNCTION PROGRAM FOR TREATING NONLOCAL POTENTIALS

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Received 6 February 1981

## PROGRAM SUMMARY

*Title of program*: NONLOCAL POTENTIALS

*Catalogue number*: ABQK

*Computer*: IBM 3032 G; *Installation*: University of Münster

*Operating system*: MVS

*Programming language used*: FORTRAN IV

*High speed storage required*: 35 180 words

*No. of bits in a word*: 32

*Overlap structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1017

*Keywords*: nonlocal potentials, partial wave expansion, scattering, bound states, Lippmann–Schwinger equation, reactance operator, half-shell, off-shell, spline functions, principal value integration

*Nature of the physical problem*
The interaction of two composite particles is often described by a nonlocal potential which (maybe for technical reasons) is available only at a finite (often sparse) set of mesh points rather than in analytic form. This situation occurs, e.g., when considering the interaction of two nuclei in the framework of a microscopic theory where antisymmetrization of the entire system is taken into account. Using a tabulation of partial-wave momentum-space matrix elements of the potential, the present program solves the scattering problem and it searches for bound states.

*Method of solution*
The Lippmann–Schwinger (integral) equation for the reactance operator [3] (i.e. the real equivalent to the $T$-matrix) is solved in momentum space utilizing cubic spline functions [2] to approximate the integrand and to treat the principal value singularity of the integral kernel. A detailed description of the algorithm used is given in ref. [1].

*Restrictions on the complexity of the problem*
Since each partial wave is treated separately the program is applicable to physical systems where only few partial waves contribute as e.g. in low-energy nuclear physics problems. Further, the number of mesh points used to discretize the potential is limited to the maximum number of coupled linear equations that can be solved with sufficient accuracy.

*Typical running time*
The execution time depends considerably on the number of discretization intervals and the number of energies the problem is solved for. The test run, with 18 discretization points and 60 energies, took 15 s.

*References*

[1] H.R. Fiebig, Comput. Phys. Commun. 20 (1980) 181.
[2] C. de Boor, A practical guide to splines, applied mathematical sciences (Springer, New York, Heidelberg, Berlin, 1978).
[3] R.G. Newton, Scattering theory of waves and particles (McGraw-Hill, New York, 1966).

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Computer Physics Communications 23 (1981) 145–152
North-Holland Publishing Company

# A CHEBYSHEV SERIES APPROXIMATION TO CONTINUOUS FUNCTIONS *

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and

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Received 4 July 1979; in revised form 19 February 1981

## PROGRAM SUMMARY

*Title of program*: CHEBY

*Catalogue number*: ABQJ

*Computer*: CDC 6600, CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: CDC SCOPE

*Programming language used*: FORTRAN IV

*High speed store required*: 8 Kwords

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of cards in combined program and test deck*: 321

*Keywords*: general purpose, Chebyshev polynomials, Chebyshev series, recurrence relations, composite trapezoidal rule integration, uniform approximation, minimax approximation, error estimate

*Nature of the physical problem*
When modelling a particular physical situation, a complicated function may be needed at many points. The function may well be very time consuming to calculate – e.g. the absorbed two-body scattering differential cross section for high-energy physics [1].

*Method of solution*
In this case it is more economical to use the original program to calculate the Chebyshev series approximation [2] to the function. Subsequent calculations will use the Chebyshev series approximation and will be fast. The program described in this paper is designed to:

(i) evaluate $N + 1$ approximate Chebyshev coefficients for a function defined on $[-1, 1]$, by using the values of that function at $M + 1$ Chebyshev points, where $M$ and $N$ ($\leqslant M$) are specified by the user;

(ii) sum a finite Chebyshev series by Clenshaw's method (also known as Goertzel's or Watt's method).

The program also contains subroutines to evaluate a particular function $F$ and to calculate errors by comparing the exact value of $F$ with the sum of the approximating finite Chebyshev series. An error estimate, based on the sum of the absolute value of the eight successive Chebyshev series coefficients beyond those used in the finite Chebyshev series summation, is also presented.

*Restrictions on the complexity of the program*
The only restrictions on the program are the number $M$ of points used in the calculation of the Chebyshev series coefficients, and the number of terms $N$ in the Chebyshev series approximation. For the accurate calculation of the coefficients, we must have $N \leqslant M$. The program is dimensioned for $N \leqslant M \leqslant 400$. This can be altered by the user. However, for an accurate calculation of the error bound we should have $N + 8 \leqslant M$ which gives the inequality $N + 8 \leqslant M \leqslant 400$.

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[*] Part of the University of London Data Handling and Data Presentation Project.

[**] Permanent address: Department of Mathematics, Royal Holloway College, Egham, Surrey, TW20 0EX, UK.

*References*

[1] P.A. Collins, B.J. Hartley, R.W. Moore and K.J.M. Moriarty, Comput. Phys. Commun. 5 (1973) 349.

[2] M.A. Snyder, Chebyshev methods in numerical approximation (Prentice Hall, New York, 1966).

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North-Holland Publishing Company

# COMPUTATION OF TOTAL CROSS-SECTIONS FOR ELECTRON CAPTURE IN HIGH ENERGY ION–ATOM COLLISIONS

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Received 1 December 1980

## PROGRAM SUMMARY

*Title of program*: CDW 1

*Catalogue number*: AAHL

*Computer*: IRIS 80; *Installation*: Centre Interuniversitaire de Calcul-Bordeaux

*Operating system*: SIRIS 10

*Other computer on which it is operable*: PDP 11

*Programming language used*: FORTRAN

*High speed storage required*: 17 Kwords

*Number of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: input and output units with records length ⩾80 characters

*No. of cards in combined program and test deck*: 948

*Keywords*: atomic collisions, electron capture

*Nature of the physical problem*
Calculate the cross-section for electron capture in a high energy ion–atom collision.

*Method of solution*
The program is based on the continuum distorted wave (CDW) method of Cheshire [1] as generalized to complex systems by the authors [2]. The initial and final orbital of the captured electron are supposed to be described by a linear combination of Slater type orbitals.

*Restriction on the complexity of the problem*
The impact energy should be greater than 80 $\sup\{|\epsilon_i|, |\epsilon_f|\}$ keV/amu where $\epsilon_i$ and $\epsilon_f$ are the initial and final orbital energies of the captured electron expressed in atomic units. The orbitals should be of the types 1s, 2s, 3s, 4s, 2p, 3p.

*Typical running time*
The running time for the test run on the IRIS 80 is 0.36 min.

*References*

[1] I.M. Cheshire, Proc. Phys. Soc. 84 (1964) 89.
[2] Dž. Belkić, R. Gayet and A. Salin, Phys. Rep. 56 (1979) 279.

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* Equipe de recherche CNRS No. 137.

## PROGRAM SUMMARY

*Title of program*: CDW 2

*Catalogue number*: AAHM

*Computer*: IRIS 80; *Installation*: Centre Interuniversitaire de Calcul, Bordeaux

*Operating system*: SIRIS 10

*Other computer on which it is operable*: PDP 11

*Programming language used*: FORTRAN

*High speed storage required*: 15 Kwords

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: input and output units with record length ⩾80 characters

*No. of cards in combined program and test deck*: 868

*Keywords*: atomic collisions, electron capture

*Nature of physical problem*
Calculate the cross-section for electron capture in a high-energy ion–atom collision.

*Method of solution*
The program is based on the continuum distorted wave (CDW) method of Cheshire [1] as generalized to complex systems by the authors [2]. The initial orbital of the captured electron is supposed to be described by a linear combination of Slater type orbitals. The final orbital is a hydrogenic one.

*Restriction on the complexity of the problem*
The impact energy should be greater than 80 sup$\{|\epsilon_i|, |\epsilon_f|\}$ keV/amu where $\epsilon_i$ and $\epsilon_f$ are the initial and final orbital energies of the captured electron expressed in atomic units. The orbitals should be of the types 1s, 2s, 3s, 4s, 2p, 3p.

*Typical running time*
The running time for the test run on the IRIS 80 is 0.64 min.

*References*

[1] I.M. Cheshire, Proc. Phys. Soc. 84 (1964) 89.
[2] Dž. Belkić, R. Gayet and A. Salin, Phys. Rep. 56 (1979) 279.

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Computer Physics Communications 23 (1981) 169–180
North-Holland Publishing Company

# THE POTENTIAL CREATED BY AN ALTERNATING POINT CHARGE IN A MAXWELLIAN MAGNETO-PLASMA

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*CNES/CST, 31055 Toulouse Cédex, France*

Received in final form 23 October 1980

## PROGRAM SUMMARY

*Title of program*: POTENT

*Catalogue number*: AAQP

*Computer:* CDC Cyber 170, model 750, simple precision; *Installation:* CNES/CST, Division Mathematiques et traitements, Toulouse

*Operating system:* NOS/BE–level 508

*Programming language used*: FORTRAN IV (H level)

*High speed storage required:* 103 Koctets

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: one

*Other peripherals used*: line printer

*No. of cards in combined program and test deck:* 426

*Keywords*: plasma physics, forced potential, point antenna, electrostatic waves

*Nature of physical problem*
Computation of the potential created by an alternating point charge in a stationary Maxwellian magneto-plasma, neglecting ion motion and collisions, for a broad range of values of the distance vector from the source and of the plasma frequency, when the excitation frequency is below the cyclotron frequency.

*Method of solution*
By using the least-damped-root approximation [1], the potential is expressed as a single integral over the field-aligned component $k_\parallel$ of the wave vector. The calculation of this integral only needs the knowledge of the least-damped root of the dispersion equation for electrostatic waves, together with its derivative, as functions of $k_\parallel$. They are obtained from a complete set of tabulated values on a magnetic tape by using a second-order Newton interpolation method.

As a first step, the values of the least-damped root and of the derivative are read from the magnetic tape, and a double interpolation is made with respect to the excitation and the plasma frequencies. Then the numerical integration is performed over successive five-point intervals by an iterative method, in which integration by Filon's method and interpolation over $k_\parallel$ by Newton's method are made together, until the required accuracy is reached. The total integral is then computed as the sum of the convergent series obtained by adding the partial integration results.

*Restrictions on the complexity of the problem*
The only restrictions of the problem are:
1) The distance from the source must be greater than 5 and less than 1000 times the Larmor radius.
2) The plasma frequency must be greater than 0.1 and less than 40 times the cyclotron frequency.
3) The angle between the distance vector and the magnetic field direction must be different from 0.

*Typical running time*
The test run output, comprising 52 values of the potential, is computed in about 276.173 s.

*Reference*
[1] L.R.O. Storey and J. Thiel, Phys. Fluids 21 (1978) 2325.

Computer Physics Communications 23 (1981) 181–198
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# ASYPCK2, AN EXTENDED VERSION OF ASYPCK

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Received 1 October 1980; in revised form 7 January 1981

## PROGRAM SUMMARY

*Title of program*: ASYPCK2, an extended version of ASYPCK

*Catalogue number*: AANK

*Reference to original program*: CPC Program library file AAJA [1]

*Author of original program*: M.A. Crees, Comput. Phys. Commun. 19 (1980) 103

*Computer*: IBM 360/195; *Installation*: Rutherford Laboratory

*Other machines on which the program has been tested*: CDC 6400, CDC 6600, CDC 7600, IBM 370/165 and CRAY-1

*Operating system*: HASP II

*Programming language used*: FORTRAN IV

*High speed storage required*: 136 kbytes (decimal)

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, lineprinter, 2 permanent disc files, 1 scratch file, card punch optional

*No. of cards in combined program and test deck*: 4398

*CPC library subprograms used*: *title*: ASYPRO2, *catalogue number*: AANL, *ref. in CPC*: this paper, section 6

*Keywords*: atomic physics, asymptotic solutions, electron–ion, electron–atom, electron–molecule, scattering, expansion methods, Fox–Goodwin integration

*Nature of the problem*
The program ASYPCK [1] (CPC Program library file AAJA) has been used extensively to obtain asymptotic solutions of the second-order differential equations of the type encountered in electron–ion and electron–atom scattering (for example in conjunction with the programs IMPACT [2] and RMATRX [3]). With increased usage a number of improvements and additional facilities have been developed and incorporated in this new version of ASYPCK, known as ASYPCK2. New features include a version for use on CRAY machines, a double precision version for use on IBM machines and an automatic setting of the Fox–Goodwin parameter MFG (see sections 5.3 and 9 of ref. [1]).

*Method of solution*
As ASYPCK [1].

*Restrictions on the complexity of the problem*
The program ASYPCK2 is provided in a form which must be pre-processed by a program ASYPRO2 (see this paper, section 6), which is an updated version of the program ASYPRO [1].

*Typical running time*
As ASYPCK [1], except that when running the special CRAY version on CRAY machines, in which case considerable time saving may be achieved.

*References*

[1] M.A. Crees, Comput. Phys. Commun. 19 (1980) 103.
[2] M.A. Crees, M.J. Seaton and P.M.H. Wilson, Comput. Phys. Commun. 15 (1978) 23.
[3] K.A. Berrington, P.G. Burke, M. Le Dourneuf, W.D. Robb, K.T. Taylor and Vo Ky Lan, Comput. Phys. Commun. 14 (1978) 367.

## PROGRAM SUMMARY

*Title of program*: ASYPRO2, an updated version of ASYPRO

*Catalogue number*: AANL

*Reference to original program*: CPC Program library file AAJB [1]

*Author of original program*: M.A. Crees, Comput. Phys. Commun. 19 (1980) 103

*Computer*: IBM 360/195; *Installation*: Rutherford Laboratory

*Other machines on which program has been tested*: CDC 6400, CDC 6600, CDC 7600, IBM 370/165 and CRAY-1

*Operating system*: HASP II

*Programming language used*: FORTRAN IV

*No. of bits in a word*: 32

*High speed storage required:* 46 kbytes (decimal)

*No. of magnetic tapes required*: none

*Other peripherals required*: card reader, line printer, one scratch file, two permanent disc files, card punch optional

*No. of cards in combined program and test deck*: 773

*Keywords*: atomic physics, pre-processor, editing, asymptotic solutions, electron–ion, electron–molecule, scattering

*Nature of the problem*
ASYPRO2 is a pre-processor for the program ASYPCK2 (this paper, catalogue number AANK). It is an updated version of the program ASYPRO [1] (catalogue number AAJB). The program can be used to pre-process the previously published program ASYPCK [1], but the published version of ASYPRO cannot be used to pre-process the program ASYPCK2. ASYPRO2 is also the pre-processor for the program ASYSLIM (this paper, section 5).

*Method of solution*
As ASYPRO [1], except that additional parameters read in as data may be required, depending on version of ASYPCK2 or ASYSLIM desired (see section 6 of this paper).

*Restrictions on the complexity of the problem*
As ASYPRO [1].

*Typical running time*
As ASYPRO [1].

*Reference*
[1] M.A. Crees, Comput. Phys. Commun. 19 (1980) 103.

## PROGRAM SUMMARY

*Title of program*: ASYSLIM, a streamlined version of ASYPCK2

*Catalogue number*: AANM

*Reference to original program*: this paper

*Author of original program*: M.A. Crees, this paper

*Computer*: IBM 360/195; *Installation*: Rutherford Laboratory

*Other machines on which program has been tested*: CDC 6400, CDC 6600, CDC 7600, IBM 370/165 and CRAY-1

*Operating system*: HASP II

*Programming language used*: FORTRAN IV

*High speed storage required*: 75 kbytes (decimal)

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals required*: card reader, line printer, two permanent disc files, card punch optional

*No. of cards in combined program and test deck*: 194

*PC subprograms used*: *titles*: ASYPCK2, ASYPRO2, *atalogue numbers*: AANK, AANL, *ref. in CPC*: this paper

*eywords*: atomic physics, asymptotic solutions, electron–on, electron–atom, electron–molecule, scattering, expan-ion methods, Fox–Goodwin integration

*ature of the problem*
The program ASYPCK2 (this paper) contains a large variety f facilities, some of which require a reasonable amount of ore. In some instances the program ASYPCK2 is run for ases which do not use all of the facilities and hence there an arise a wastage of core. A streamlined version of ASYPCK2 has been developed, removing some of the features and methods of the program, but which can require considerably less high speed storage. This streamlined version of ASYPCK2 is known as ASYSLIM, and is produced from AANK using AANM as an adaptation deck.

*Method of solution*
As ASYPCK [1].

*Restrictions on the complexity of the problem*
The program ASYSLIM is provided in a form which must be pre-processed by the program ASYPRO2 (this paper, section 6).

*Typical running time*
As ASYPCK2 [2].

*References*

[1] M.A. Crees, Comput. Phys. Commun. 19 (1980) 103.
[2] M.A. Crees, this paper.

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Computer Physics Communications 23 (1981) 199–207
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# SATDSK: A NUMERICAL SIMULATION OF THE MAGNETIC FIELD DUE TO SATURATED IRON IN CYCLOTRON POLETIPS

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*Oak Ridge National Laboratory* *, *Union Carbide Corporation, Nuclear Division, Oak Ridge, TN 37830, USA*

Received 1 August 1980

## PROGRAM SUMMARY

*Title of program*: SATDSK

*Catalogue number*: ABKI

*Computer*: IBM 360/91; *Installation*: Oak Ridge National Laboratory, Oak Ridge, Tennessee

*Operating system*: MVT

*Programming language used*: FORTRAN IV

*High-speed storage required*: 144 kbytes

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1286

*Keywords*: magnetic fields, uniform magnetization, saturated iron, cyclotrons

*Nature of physical problem*
The program calculates the magnetic field due to uniformly magnetized iron poletips, with symmetries appropriate for cyclotron design studies.

*Method of solution*
The assumption of uniformly magnetized iron reduces the field calculation from one of three-dimensional volume integrals to two-dimensional surface integrals, with corresponding reductions in running time and array sizes, as well as reduced complexity of input parameters. The uniform magnetization assumption is quite appropriate for high magnetic fields which would be found in many recent superconducting cyclotron designs.

*Restrictions on the complexity of the problem*
Fields are calculated only in the median plane for median-plane-symmetric iron poletips.

*Typical running time*
Approximately 0.15 s per field point.

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* Operated by Union Carbide Corporation, Nuclear Division under contract W-7405-eng-26 for the US Department of Energy.

Computer Physics Communications 23 (1981) 209–220
North-Holland Publishing Company

# MANUAL FOR COMMUTE, A FORTRAN PROGRAM FOR SYMBOLIC EVALUATION OF COMMUTATORS AND CORRELATION FUNCTIONS

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and

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Received 20 June 1980; in revised form 3 April 1981

## PROGRAM SUMMARY

*Title of program*: COMMUTE

*Catalogue number*: ACKS

*Computer*: IBM 3033, IBM 370/168, PDP 11/45, VAX 11/780

*Operating system*: OS/MVS/, RSX-11/D, VAX/VMS V2.1

*Programming language used*: FORTRAN IVH EXTENDED, FORTRAN IV PLUS

*High speed storage required*: 300 K (IBM), 32 K (PDP, VAX)

*No. of bits in a word*: 32 (IBM, VAX), 16 (PDP)

*Overlay structure*: no (IBM, VAX) yes (PDP)

*No. of magnetic tapes required*: none

*Other peripherals used*: DISK

*No. of cards in combined program and test deck*: 5219

*Keywords*: many body theory, equations of motion, correlation functions, symbolic evaluation

*Nature of the physical problem*
COMMUTE is a FORTRAN program that can be used for the symbolic evaluation of equations of motion of operators or correlation functions. It can use symmetry operations to reduce the final number of terms and in some specific cases, it expresses correlation functions in terms of known functions. It is extremely useful for the calculation of the coefficients in the short-time expansion of a correlation function.

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* Supported by the IIKW project "Neutronenverstrooiing".
** Aspirant of the "Belgisch Nationaal Fonds voor Wetenschappelijk Onderzoek".

Computer Physics Communications 23 (1981) 221
North-Holland Publishing Company

## ERRATUM NOTICE

*Title of manuscript*: A program for perspective views of three-dimensional surfaces

*Authors*: E.A. Olszewski and W.J. Thompson

*Reference*: Comput. Phys. Commun. 21 (1980) 185

*Title of program*: TDPLOT3

*Catalogue number*: ABVL

*Title of manuscript*: A program to calculate transverse Breit and QED corrections to energy levels in a multiconfiguration Dirac–Fock environment

*Authors*: B.J. McKenzie, I.P. Grant and P.H. Norrington

*Reference*: Comput. Phys. Commun. 21 (1980) 233

*Title of program*: MCBP/BENA

*Catalogue number*: AAND

Computer Physics Communications 23 (1981) 233–273
North-Holland Publishing Company

# A GENERAL PROGRAM TO CALCULATE ATOMIC CONTINUUM PROCESSES USING THE NIEM METHOD

Ronald J.W. HENRY, S.P. ROUNTREE * and Ed R. SMITH
*Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA*

Received 8 October 1980

This paper describes a set of computer program packages NIEM which enable electron–atom and electron–ion collision cross sections to be calculated for a general atomic system described by *LS*-coupling. The calculations are based on a non-iterative integral equation method.

## PROGRAM SUMMARY

*Title of program*: NIEM POTC1

*Catalogue number*: AAJG

*Computer*: IBM 3033; *Installation*: Systems Network Computer Center, Louisiana State University, Baton Rouge, LA 70803, USA

*Operating system*: JES2

*Programming language used*: FORTRAN IV

*High speed store required*: 232 K

*Number of bits per word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, scratch disc store, permanent disc store

*Number of cards in combined program and test deck*: 6393

*CPC library subprograms used*

| *Cat. no.* | *Title* | *Ref. in CPC* | *No. of cards* |
|---|---|---|---|
| AAJH | NIEM NIES2 | this paper | 3162 |
| AAJI | NIEM ASYM3 | this paper | 2086 |
| ACWN0001 | GRN2 | this paper | 2220 |

*Keywords*: atomic, electron atom scattering, electron ion scattering, non-iterative integral equation method

*Nature of the physical problem*
This program calculates all the interaction potentials involving the bound and continuum electrons necessary to enable electron atom or electron ion scattering to be calculated for a general atomic system. The bound orbitals are specified analytically. Direct potentials, the coefficients in the asymptotic expansion of the potentials, exchange coefficients and correlation potentials are stored on a permanent tape or disc file for use by NIEM NIES2 [1].

*Method of solution*
The one-electron integrals and the multiple integrals are evaluated numerically using the trapezoidal rule. The triangular relations are used to determine the number of coupled channels given the quantum numbers of the target and scattering states. The angular integrals are carried out using the methods of Racah algebra.

*Restrictions on the complexity of the program*
Up to 10 bound orbitals and 6 scattering channels for each total angular momentum can be included. Larger calculations can be made by recompiling with larger dimensions. Instructions on comment cards are given to enable the user to increase the dimensions. Normal output includes the dimension size currently used and the size allocated. *LS* coupling is assumed.

*Typical running time*
The test runs took 12.4 and 42.9 s on the IBM 3033.

*Reference*

[1] R.J.W. Henry, S.P. Rountree and E.R. Smith, Comput. Phys. Commun., this paper.

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* Present address: Digitran, 501 Industrial Parkway, Lafayette, LA 70501, USA.

## PROGRAM SUMMARY

*Title of program*: NIEM NIES2

*Catalogue number*: AAJH

*Computer*: IBM 3033; *Installation*: Systems Network Computer Center, Louisiana State University, Baton Rouge, LA 70803, USA

*Operating system*: JES2

*Program language used*: FORTRAN IV

*High speed storage required*: 252 K

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, scratch disc store, permanent disc store

*Number of cards in combined program and test deck*: 3162

*CPC library subprograms used*:

| *Cat. no.* | *Title* | *Ref. in CPC* | *No. of cards* |
|---|---|---|---|
| AAJG | NIEM POTC1 | this paper | 6393 |
| AAJI | NIEM ASYM3 | this paper | 2086 |
| ACWN0001 | GRN2 | this paper | 2220 |

*Keywords*: atomic, close-coupling, scattering, cross section, electron, positron, atom, ion, coupled integro–differential equation, excitation, continuum wave function

*Nature of the physical problem*

This program reads the direct potentials, the coefficients in the asymptotic expansion of the potentials, exchange coefficients, and correlation potentials stored on a permanent tape or disc file by NIEM POTC1 [1]. It solves the set of integro–differential equations by a non-iterative integral equation method [2] from the origin to a radial boundary RISTOP. The program calls GRN2 [1] which calculates the regular and irregular Green's function for the problem.

*Method of solution*

The continuum orbitals are determined by using a non-iterative integral equation method [3] to propagate separately the numerator and denominator of the reactance function.

*Restrictions on the complexity of the program*

Essentially determined by NIEM POTC1 [1]. Dimensions are set for 80 particular solutions. Larger calculations can be made by recompiling with larger dimensions, which should be

## PROGRAM SUMMARY

*Title of program*: NIEM ASYM3

*Catalogue number*: AAJI

*Computer*: IBM 3033; *Installation*: Systems Network Computer Center, Louisiana State University, Baton Rouge, LA 70803, USA

*Operating system*: JES2

*Programming language used*: FORTRAN IV

*High speed core required*: 232 K

*Number of bits per word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 2086

*CPC library subprograms used*

| *Cat. no.* | *Title* | *Ref. in CPC* | *No. of cards* |
|---|---|---|---|
| ACWN0001 | GRN2 | this paper | 2220 |

done consistently with those used in NIEM POTC1 [1].

Instructions on comment cards are given to enable the user to increase the dimensions.

*Typical running time*
The test runs took 66.6 and 55.2 s on the IBM 3033.

*References*

[1] R.J.W. Henry, S.P. Rountree and E.R. Smith, Comput. Phys. Commun., this paper.
[2] W.N. Sams and D.J. Kouri, J. Chem. Phys. 51 (1969) 4809.
[3] E.R. Smith and R.J.W. Henry, Phys. Rev. A7 (1973) 1585.

*Keywords*: atomic, electron atom scattering, electron ion scattering, asymptotic solutions, reactance matrices

*Nature of the physical problem*
Reactance $K$-matrices at infinity are calculated from Wigner $R$-matrices or reactance $K$-matrices which are given at a radial boundary R1STOP, either by the user or are passed by NIEM NIES2 [1].

*Method of solution*
An integral equation method [2,3] is used to solve the coupled differential equations from R1STOP to a larger radial boundary R2STOP. The regular and irregular Green's functions for the method are calculated by GRN2 [1]. A projection method [3] is used to obtain the $K$-matrix elements at infinity from those calculated at R2STOP.

*Restriction on the complexity of the program*
Up to six scattering channels for each total angular momentum can be included. Larger calculations can be made by recompiling with larger dimensions.

*Typical running time*
The test run took 0.80 s on the IBM 3033.

*References*

[1] R.J.W. Henry, S.P. Rountree and E.R. Smith, Comput. Phys. Commun., this paper.
[2] W.N. Sams and D.J. Kouri, J. Chem. Phys. 51 (1969) 4809.
[3] E.R. Smith and R.J.W. Henry, Phys. Rev. A7 (1973) 1585.

## ADAPTATION SUMMARY

*Title of adaptation*: GRN2

*Catalogue number*: ACWN0001

*Computer*: IBM 3033; *Installation*: Systems Network Computer Center, Louisiana State University, Baton Rouge, LA 70803, USA

*Operating system*: JES2

*Programming language used*: FORTRAN IV

*High speed storage required*: 104 K

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 2220

*Reference to original program*:

*Catalogue number*: ACWN; *Title*: GRN1; *Ref. in CPC*: 11 (1976) 27

*Authors of original program*: S.P. Rountree, T. Burnett, R.J.W. Henry and C.A. Weatherford

*Keywords*: Green's functions, Ricatti–Bessel, modified Ricatti–Bessel, Coulomb functions, Whittaker functions

*Nature of the physical problem*

The subroutine GRN2 calculates Green's function solutions to a one-dimensional differential equation and returns $F_l(\rho)$ and $G_l(\rho)$, where $\rho = kr$. It differs with program GRN1 [1] in that the subroutines have been recoded to extend the range of values to large residual charge $z$ of the target and to effect time savings. The program has been modified to start at any given radial value R1STOP and it will produce $F_l(\rho)$ and $G_l(\rho)$ at any interval size specified and in blocks of NPTS steps, up to a maximum radial value of R2STOP. Four subroutines POWERD, POWERH, POWERE and POWERF have been added to evaluate, respectively, an asymptotic expansion for cases (1)–(4), i.e., $Z = 0, E > 0$; $Z = 0, E < 0$; $Z > 0, E > 0$; and $Z > 0, E < 0$.

The asymptotic expansion for cases (1) and (3) is given by [2]:

$$F_l(\rho) = \sum_{n=0}^{\infty} [g_n(\rho, \eta, l) \cos\theta_l(\rho) + f_n(\rho, \eta, l) \sin\theta_l(\rho)] ,$$

$$G_l(\rho) = \sum_{n=0}^{\infty} [f_n(\rho, \eta, l) \cos\theta_l(\rho) - g_n(\rho, \eta, l) \sin\theta_l(\rho)] ,$$

where

$$\theta_l(\rho) = \rho - \eta \ln(2\rho) - l\pi/2 + \sigma_l ,$$

$$f_0 = 1 , \quad g_0 = 0 ,$$

$$\left.\begin{aligned} f_{n+1} &= a_n f_n - b_n g_n \\ g_{n+1} &= a_n g_n + b_n f_n \end{aligned}\right\} \quad n = 0, 1, 2, \dots .$$

and

$$a_n = \frac{(2n+1) - \eta}{(2n+2)\rho} ; \qquad b_n = \frac{l(l+1) - n(n+1) + \eta^2}{(2n+2)\rho} .$$

The asymptotic expansion for cases (2) and (4) is given by [2]:

$$F_l(\rho) = \frac{1}{\sqrt{2}} e^{\rho} (2\rho)^{\eta} \sum_{n=0} c_n (2\rho)^{-n} ,$$

$$G_l(\rho) = -\frac{1}{\sqrt{2}} e^{-\rho} (2\rho)^{-\eta} \sum_{n=0} D_n (2\rho)^{-n} ,$$

where

$$\left.\begin{aligned} nC_n &= (\eta - l - n)(\eta + l - n + 1)\, C_{n-1} \\ nD_n &= -(\eta + l + n)(\eta - l + N - 1)\, D_{n-1} \end{aligned}\right. \quad n = 1, 2, 3, \dots$$

and

$$C_0 = D_0 = 1 .$$

*Restrictions on the complexity of the problem*

The order of the Green's function is restricted to $l \leqslant 50$. The arrays used in storage of the power series coefficients must be increased for $l > 50$. The program has been tested for $\eta \leqslant 0$ only, i.e., for neutral or attractive Coulomb potentials. The program can be used for all positive and negative energies except for energies which can be written in the form $E = -z^2 n^{-2}$, where $n$ is a positive integer. While the program can be called at any $\rho$, it has been tested primarily for initial values which are at either small $\rho$ where a power series expansion is valid, or in the asymptotic region where an asymptotically divergent series is used.

*Input data*

The input data is described on comment cards in the main program. The second card of the input data differs from that used for program GRN1. The second card for program GRN2 s as follows:

. ITEST, L, NPTS, R1STOP, R2STOP, ENERGY, CHARGE
ITEST, L, ENERGY and CHARGE are as described in GRN1,
NPTS number of steps required at one time,
R1STOP initial radial value,
R2STOP final radial value.

Example: If there are 121 steps from R1STOP to R2STOP and NPTS = 50, then the program will give the first 50 values of $F_l(\rho)$ and $G_l(\rho)$, then the next 50 values, and finally the remaining 21 values.

*Flow diagram*

A flow diagram for GRN2 is given in fig. 1. The values used for the discrimination TST1 is $15 + 4|\eta|/3 + l/10$. The value used for discrimination TST2 is $7 - l + 1 + 7|\eta|$.

*References*

[1] S.P. Rountree, T. Burnett, R.J.W. Henry and C.A. Weatherford, Comput. Phys. Commun. 11 (1976) 27.
[2] M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions (US Department of Commerce, N.B.S., Applied Mathematics Series 55, 1965).

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Computer Physics Communications 23 (1981) 275–286
North-Holland Publishing Company

# PSEUDOPOTENTIAL MATRIX ELEMENTS IN THE GAUSSIAN BASIS

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Received 26 November 1980

## PROGRAM SUMMARY

*Title of program*: PSEPOT

*Catalogue number*: AAQL

*Computer*: IBM 370/135; *Installation*: Institute of Information Theory and Automation, Prague, Czechoslovakia

*Operating system*: OS/VS1

*Programming language used*: FORTRAN IV

*High speed storage required*: 10 Kwords

*No. of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 971

*Keywords*: pseudopotential, matrix element, Gaussian, atom, molecule, cluster, quantum chemistry, LCAO, expansion, elementary integral

## PROGRAM SUMMARY

*Title of the program*: PSEPO1

*Catalogue number*: AAQM

*Program obtainable from*: CPC Program Library, Queen's

*Nature of the physical problem*
The incorporation of atomic pseudopotentials in the calculation of the electronic structure of molecules and larger complexes leads to a decrease in the size of the problem since in the frozen core approximation only valence electrons need to be considered. PSEPOT is a subprogram that computes matrix elements of atomic pseudopotentials occurring in the above mentioned calculations provided that both the pseudopotentials and the basis functions are expressed as linear combinations of different Gaussians.

*Method of solution*
The rather complex expression for the pseudopotential matrix elements can be decomposed into a linear combination of the products of different more or less elementary integrals. The final result is obtained roughly speaking by performing a sequence of scalar products arranged in such a manner that no more extensive calculation must be repeated twice.

*Restrictions on the complexity of the problem*
Largest pseudopotential orbital angular momentum $L_{\max} \leqslant$
Largest basis-orbital angular momentum $n_{\max} = 3$.

*Typical running time*
The running time depends considerably on the values of the angular momenta involved and on the number of Gaussians i the pseudopotential expansion. The average value for the tes run was 3.6 s per matrix element.

*Unusual features of the program*
A set of 6480 angular integrals were precalculated and placed in a few DATA statements.

*Computer*: IBM 370/135; *Installation*: Institute of Information Theory and Automation, Prague, Czechoslovakia

*Operating system*: OS/VS1

*Programming language used*: FORTRAN IV

*High speed storage required*: 9 Kwords

*No. of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, direct-access devices such as disks

*No. of cards in combined program and test deck*: 958

*CPC library program used*:
*Cat. no.*: AAQN, *Title*: COMPANGI; *Ref. in CPC*: this paper

*Reference to other published version of this program*: PSEPO1 is a more general version of PSEPOT that is also described in this paper

*Keywords*: pseudopotential, matrix element, Gaussian, atom, molecule, cluster, quantum chemistry, LCAO, expansion, elementary integral, direct-access device

*Nature of the physical problem*
The same as for PSEPOT.

*Method of solution*
The same as for PSEPOT.

*Restrictions on the complexity of the problem*
Largest pseudopotential orbital angular momentum $L_{max} \leqslant 5$.
Largest basis-orbital angular momentum $n_{max} \leqslant 5$.

*Typical running time*
The average value for the same test data as for PSEPOT increased to 9.7 s per matrix element.

*Unusual features of the program*
In this case the set of angular integrals, whose number may increase up to 243936, are stored in a permanent direct-access disk file. This file is created by the program COMPANGI, that has to be run prior to the use of PSEPO1. In addition some intermediate data are stored in other disk files.

## PROGRAM SUMMARY

*Title of program*: COMPANGI

*Catalogue number*: AAQN

*Computer*: IBM 370/135; *Installation*: Institute of Information Theory and Automation, Prague, Czechoslovakia

*Operating system*: OS/VS1

*Programming language used*: FORTRAN IV

*High speed storage required*: 3 Kwords

*No. of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, direct-access device such as disk

*No. of cards in combined program and test deck*: 249

*Keywords*: angular integral, data initialization, expansion

*Nature of the physical problem*
Computation of angular integrals for the program PSEPO1

*Method of solution*
Appropriate expansion of real spherical harmonics leads to analytically evaluable integrals.

*Restrictions on the complexity of the problem*
Compatible with those for PSEPO1.

*Typical running time*
27 s for $L_{max} = 2$, $n_{max} = 3$; 17 min for $L_{max} = n_{max} = 5$.

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Computer Physics Communications 23 (1981) 287–299
North-Holland Publishing Company

# SPLINE INTERPOLATION AND SMOOTHING OF DATA

R.E. CUTKOSKY and C. POMPONIU *
*Physics Department, Carnegie-Mellon University, Pittsburgh, PA 15213, USA*

Received 17 November 1980

## PROGRAM SUMMARY

*Title of program*: SPLINESMOOTH

*Catalogue number*: AAQO

*Computer*: DEC VAX 11/780; *Installation*: Department of Physics, Carnegie-Mellon University, Schenley Park, Pittsburgh, PA 15213, any other computer having a FORTRAN IV compiler

*Programming language used*: FORTRAN IV

*High speed storage required*: 33 152 words + FORTRAN LIBRARY

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: magnetic disk, printer

*No. of cards in combined program and test deck*: 832

*Keywords*: approximation, smoothing, splines, $\chi^2$-fit, orthogonalization, constrained optimization

*Nature of the physical problem*
In many branches of physics, a recurrent problem is that of smoothing a set of experimental data, measured at a sequence of values of some independent variable. This is done as a first step towards interpolating, integrating, differentiating, or otherwise transforming the function represented by the data. Sometimes a suitable family of theoretically motivated functions can be used to fit the data; in other more general cases, it is convenient to use functions which have a general character. We present here a method which uses spline functions for smoothing a given set of data. The use of splines is suggested by the well-known utility of these functions for interpolating data given without error, but in the presence of errors different techniques for their construction are required in order to preserve statistical and numerical stability.

*Method of solution*
A sequence of expansion functions is generated by applying the spline kernel to "seed functions". A stiffness parameter determines the truncation of the expansion (and also enters into their recurrence relations). The value of the stiffness parameter can be assigned on an a priori basis, or it can be adjusted in accordance with the maximum-likelihood principle.

*Restrictions on the complexity of the problem*
The data depend on only one independent variable, and are assumed to have uncorrelated errors.

*Typical running time*
With 100 data points and 18 vectors, the running time was 13 s for one pass, and 0.5 s for each subsequent iteration.

*Unusual features of the program*
For each new stiffness value, the corresponding orthonormal basis is constructed by rotating the previous one, thus saving time while preserving accuracy.

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* Present address: Exxon Production Research Co., P.O. Box 2189, Houston, TX 77001, USA.

Computer Physics Communications 23 (1981) 301–305
North-Holland Publishing Company

# A MICROCOMPUTER PROGRAM FOR THE CORRELATING OF TWO ORDERED LISTS OF NUMBERS *

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Received 1 August 1980; in revised form 2 April 1981

## PROGRAM SUMMARY

*Title of program*: INDCAL

*Catalogue number*: AAQR

*Computer*: DEC PDP-11/03 (and up); *Installation*: University of Windsor

*Operating system*: RT-11

*Programming language used*: PDP Assembler, (Fortran driver available)

*High speed storage required*: 878 words

*No. of bits in a word*: 16

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 550

*Keywords*: unitary group, spectroscopy, ordered lists, microcomputer, assembler

*Nature of the physical problem*
The program segment determines the positions of different entries in two ordered lists of numbers. This is done for the analysis of complex spectra using the Unitary Group methods.

*Method of solution*
Iterative 'compare' statements.

*Restrictions on the complexity of the problem*
As given, the program treats only cases where, at most, two entries differ.

*Typical running time*
Depending on the length of the list to be analyzed. Typically for 10 numbers, 10–15 ms.

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Computer Physics Communications 23 (1981) 307–335
North-Holland Publishing Company

# PROGRAM SYSTEM FOR ANALYSING POSITRON LIFETIME SPECTRA AND ANGULAR CORRELATION CURVES

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*Computer Installation, Risø National Laboratory, DK-4000 Roskilde, Denmark*

Morten ELDRUP, Ole E. MOGENSEN and Niels J. PEDERSEN
*Chemistry Department, Risø National Laboratory, DK-4000 Roskilde, Denmark*

Received 1 March 1981

## PROGRAM SUMMARY

*Title of program system*: PATFIT consisting of the four programs POSITRONFIT, RESOLUTION, PAACFIT and PARAFIT

*Catalogue number*: AANN

*Computers*: Burroughs 6700, CDC CYBER 173; *Installation*: RISØ, Denmark, RECAU, Aarhus, Denmark

*Operating systems*: Burroughs B6700 MCP Mark III.0.1, CDC NOS. VER. 1.4-509/508-A

*Programming language used*: FORTRAN 77 * for the CDC version

*High speed storage required*: POSITRONFIT 48000, RESOLUTION 70000, PAACFIT 37000, PARAFIT 34000 words

*No. of bits per word*: minimum 48

*Overlay structure*: none

*No. of tapes required*: none

*Other peripherals used*: input from card reader/remote terminal/disk file, output on lineprinter

*No. of cards in combined program system and test deck:* 5599

*Reference to other published versions of part of this program system*:

| *Catalogue no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAGK | POSITRONFIT | 3 (1972) 240 |
| AAGX | POSITRONFIT EXTENDED | 7 (1974) 401 |
| AAGZ | DBLCON | 13 (1978) 371 |
| AAHI | INTERACTIVE POSITRONFIT | 15 (1978) 97 |

*Keywords*: positron annihilation, lifetime, angular correlation, time spectrum, angular correlation curve, least squares, fitting, convolution, resolution function, minimization, Marquardt, constraints, correlation matrix

*Nature of the physical problem*
In the field of positron annihilation research two of the experimental methods used are positron lifetime and angular correlation measurements. In both cases a measured spectrum normally consists of a sum of several components. The experimenter wants to extract from the spectra characteristic parameters for each component.

*Method of solution*
A measured spectrum is fitted with a mathematical model by a constrained semilinear least-squares technique. This results in estimates of the model function parameters.

*Restriction on the complexity of the programs*
There are certain limitations on the number of fitting parameters and data points, which are listed in the context of the four programs.

*Typical running time*
(CYBER 173 CPU-seconds for the test cases) POSITRONFIT: 8.4 s, RESOLUTION: 9.8 s, PAACFIT: 3.2 s, PARAFIT 3.1 s

* A FORTRAN IV version of the package for the B6700 computer at Risø can be obtained from the authors.

Computer Physics Communications 23 (1981) 355–364
North-Holland Publishing Company

# DESIGN AND IMPLEMENTATION OF A WORD ADDRESSABLE DATA SET FOR DEC-10 COMPUTERS *

B.C. KARP and J.R. COMFORT

*Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA*

Received 31 March 1981

## PROGRAM SUMMARY

*Title of program*: WORD ADDRESSABLE DATA SET

*Catalogue number*: AAQS

*Computer*: DEC-1099; *Installation*: University of Pittsburgh, Pittsburgh, Pennsylvania

*Operating system*: TOPS-10

*Programming language used*: MACRO-10

*High speed storage required*: Subroutine package contains 806 words; subroutine package allocates at least an additional 128 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: disk; line printer or output terminal

*No. of cards in combined program and test deck*: 1457

*Keywords*: General purpose, utility, word-addressable data sets, disk organization, random/sequential I/O, file structures

*Nature of physical problem*

It is convenient to have available a Fortran-callable subroutine package to perform random access I/O to or from an external device. I/O should be as efficient as possible and still provide flexibility in accessing information.

*Method of solution*

For DEC-10 computers, a subroutine package implements a word addressable data set (WADS) concept. Design and implementation has been guided by the organization of the WADS available on CDC computers through the CDC Record Manager Package [1].

*Restriction on the complexity of the problem*

User's programs must allocate a 20 word "file information table" (FIT). More than one data set may be open simultaneously, but a separate FIT is required for each. Data sets are limited in length to about $2^{25}$ words.

*Unusual features of the program*

The subroutine package allocates a software I/O channel and core for an I/O buffer from the DEC Fortran-10 I/O package FOROTS.

*References*

[1] CYBER Record Manager Version 1 Reference Manual, Control Data Corporation (1977).

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* Supported in part by the National Science Foundation.

Computer Physics Communications 23 (1981) 365–375
North-Holland Publishing Company

# IMPLEMENTATION OF THE PARTITIONED DATA SET CONCEPT FOR DEC-10 COMPUTERS [*]

B.C. KARP and J.R. COMFORT
*Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260, USA*

Received 1 April 1981

## PROGRAM SUMMARY

*Title of program*: DEC-10 PARTITIONED DATA SETS

*Catalogue number*: AAQT

*Computer*: DEC-1099; *Installation*: University of Pittsburgh, Pittsburgh, Pennsylvania

*Operation system*: TOPS-10

*Programming language used*: DEC FORTRAN-10, MACRO-10

*High speed storage required*: 2503 words in subroutine package; main program requires 5788 words; Blank subroutines require 177 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none required; at least one optional

*Other peripherals used*: disk; line printer

*No. of cards in combined program and test deck*: 1697

*CPC library subprograms used*
*Catalogue number*: AAQS; *Title*: WADS; *Ref. in CPC*: 19 (1980) 51.

*Keywords*: general purpose, utility, partitioned data sets, disk organization, file structures, random/sequential I/O, libraries, card-image storage

*Nature of the physical problem*
User's programs may need to make input/output to numerous sets of similar data, each to be read sequentially but in an order to be determined at execution time. It is convenient to group sets of data into a single data set on a random-access device and arrange for the sequential transfer of the data for an individual "member". Documentary information and back-up capacities may also be desired. A significant savings in storage space can be obtained if multiple blanks are removed from character data, and replaced when the data are read.

*Method of solution*
For DEC-10 computers, a subroutine package implements a "partitioned data set" (PDS) concept [2] on a word addressable data set (WADS) [3]. For card-image applications, program MANAGR is a handy utility program for data storage, retrieval and documentation. Another subroutine package removes and later restores occurrences of multiple blanks in character data.

*Restrictions on the complexity of the problem*
User's programs must allocate core for PDS directories and file-information tables. I/O may be made with only one member of a PDS at a time. The total length of the data set is limited to about $2^{25}$ words. Program MANAGR is restricted to working with card-image data (readable under alphanumeri format in Fortran). There may be no more than 400 members of a PDS.

*Unusual features of the program*
A DATE routine must be added to the MANAGR program deck.

*References*

[1] J.R. Comfort, Comput. Phys. Commun. 19 (1980) 51.
[2] J.R. Comfort, Comput. Phys. Commun. 19 (1980) 43.
[3] B.C. Karp and J.R. Comfort, Comput. Phys. Commun. 23 (1981) 355.

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[*] Supported in part by the National Science Foundation.

Computer Physics Communications 23 (1981) 377–384
North-Holland Publishing Company

# COMPUTATION OF FOURIER TRANSFORM OF A GENERAL TWO-CENTRE STO CHARGE DISTRIBUTION

B.R. JUNKER *
*Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA*

Received 16 July 1980; in revised form 1 December 1980

## PROGRAM SUMMARY

*Title of Program*: FRTRF

*Catalogue number*: AANO

*Computers*: IBM 360 and 370 series (CDC although double precision should be converted to single precision); *Installation*: Oak Ridge National Laboratory and Goddard Space Flight Center

*Operating system*: MVT

*Programming language used*: FORTRAN IV

*High speed storage required*: 57416 bytes

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 540

*Keywords*: charge transfer, Bethe theory, coherent X-ray scattering, Fourier transform, Bessel functions

*Nature of physical problem*
The computation of the charge tranfer amplitude at energies greater than a few keV's requires the computation of two-centre integrals of the form of Fourier transforms. Similar integrals arise in the Bethe theory of the scattering of charged unstructured particles by molecules and in the computation of the coherent and incoherent intensities of X-rays scattered by molecules. This program provides a means of computing these integrals for an arbitrary Slater Type Orbital (STO) basis.

*Method of solution*
The technique is a generalization to STO's with arbitrary quantum numbers of McCarroll's method [1] for s-orbitals.

*Restrictions on program*
The restrictions on the program are determined only by the dimensions of the arrays. As written, the maximum quantum numbers allowed are $n = 5$, $l = 5$, $m = 5$, and the maximum number of quadrature points is fifty. These restrictions can be relaxed by increasing the appropriate dimension declarations.

*Typical running time*
A number of test runs were performed to determine the variation of run time with respect to the various parameters. In all runs the complete set of integrals was computed at an internuclear separation of 1.0 au with an impact parameter of 0.5 au and at an internuclear separation of 5.0 au with an impact parameter of 1.5 au. Two different basis sets were used – one contained 1s, 2s, $2p_0$ and $2p_{\pm 1}$ STO's on each center while the other contained $3d_0$, $3d_{\pm 1}$, $3d_{\pm 2}$, $3f_0$, $3f_{\pm 1}$, $3f_{\pm 2}$ and $3f_{\pm 3}$ in addition to the orbitals of the first set. In both cases, the nonlinear parameters were chosen to correspond to a hydrogen atom for center A and a hydrogenlike helium ion for center B. The first basis set resulted in the computation of 150 integrals while the second required 1734 integrals. In the first set of runs CONV was set to $2 \times 10^{-6}$ and VEL to 2.5 au. The first basis set required 32 ms/integral when the first 26 points of a 64 Gauss–Laguerre quadrature set was used, 40 ms/integral for the first 50 of 96 point s, and 56 ms/integral for 50 of 128. The second basis set required 99 ms/inte-

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gral for 50 of 96 and 111 ms/integral for 50 of 128. When VEL was set to 0.25 au, the first basis set required 36 ms/integral for 50 of 96, while the second required 88 ms/integral for 50 of 96 and 94 ms/integral for 50 of 128. When CONV was set to $2 \times 10^{-8}$ and VEL to 2.5 au, the first basis set required 44 ms/integral for 50 of 96 and 56 ms/integral for 50 of 128, while the second basis set required 121 ms fo 50 of 128.

## *References*

[1] R. McCarroll, Proc. Roy. Soc. A246 (1961) 547.

Computer Physics Communications 23 (1981) 385–391
North-Holland Publishing Company

# EFFY, A PROGRAM TO CALCULATE THE COUNTING EFFICIENCY OF BETA PARTICLES IN LIQUID SCINTILLATORS

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Received 4 May 1981

## PROGRAM SUMMARY

*Title of program*: EFFY

*Catalogue number*: ABQL

*Computer*: UNIVAC 1100/80; *Installation*: Centro de Cálculo, Junta de Energía Nuclear, Ciudad Universitaria, Madrid, Spain

*Operating system*: EXEC 8

*Programming language used*: FORTRAN IV

*High speed storage required*: 20 kbytes (decimal)

*No. of bits in byte*: 36

*Overlay structure*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 419

*Keywords*: beta spectra, beta decay, efficiency

*Nature of the physical problem*
In liquid scintillation counting it is often required to know the counting efficiency. A model of the basic interactions allows one to calculate the detection efficiency for beta emitters as a function of the figure of merit. The program is applicable to single and complex beta emitters.

*Method of solution*
The beta spectrum is calculated from the Fermi theory of beta decay. Corrections by a shape factor have been considered. The total detection probability is obtained by dividing the spectrum into bands, calculating the detection probability for each band and summing.

*Restrictions on the complexity of the problem*
The program is designed to be used in the counting efficiency calculation of negatron and positron emitters. The counting efficiency computation for electron capture nuclides is not considered. The present version of the program is restricted to spectra with 800 points. This value may be increased by increasing the storage of the corresponding arrays.

*Typical running time*
The test requires about 9 s of UNIVAC 1100/80 cpu time.

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North-Holland Publishing Company

# A COMPUTER PROGRAM FOR NUCLEAR LIFETIMES MEASUREMENTS BY DSAM USING A SELF-SUPPORTING TARGET

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Received 17 February 1981

## PROGRAM SUMMARY

*Title of program*: DSAMER

*Catalogue number*: ABQM

*Computers*: CDC 6600 and CYBER 172; *Installations*: Centre de Calcul de Physique Nucléaire, Halle aux Vins, 11, Quai Claude Bernard, 75230-Paris Cedex 5, France, Grenoble Terminal

*Operating system*: NOS/BE 1

*High speed storage required*: 3500 words

*Number of bits in a word*: 60

*Overlay structure*: none

*Peripherals used*: 1 disk pack or 1 magnetic tape

*Number of cards in combined program and test deck*: 1322

*Keywords*: Nuclear $\gamma$ spectroscopy, nuclear level lifetimes, Doppler shift attenuation method, line shape fit, nuclear stopping powers, recoiling nuclei velocity: $\beta = 1\%$ single experimental $\gamma$ spectra

*Nature of physical problem*
DSAM for nuclear lifetime measurements needs accurate nuclear stopping powers. Using self supporting targets and know long-lived levels, DSAM satisfies that condition and thus provides rather good lifetime measurements.

*Method of solution*
For given lifetime and stopping powers, the line shape of the Doppler distorted $\gamma$-ray is built up by taking into account successively the

- particle evaporation (n, p, $\alpha$),
- slowing-down of the recoiling nuclei in the target,
- different feeding laws of the studied levels,
- energy response of the GeLi detector used (including solid angle correction).

The best fit of the experimental line is chosen by the chi-square criterion.

*Restrictions on the complexity of the problem*
- Number of evaporated particles must be $\leqslant 3$, ($2\alpha$ maximum),
- range of lifetime measurements: $0.02 \text{ ps} < \tau < 5 \text{ ps}$,
- typical recoiling ions initial velocity: $\beta = 1\%$, typical nuclei mass and target: $50 < A < 80$, typical target thickness: $1 \text{ mg/cm}^2$,
- number of mixed $\gamma$ rays to be analyzed must be $\leqslant 2$.

*Typical running time*
About 1/2 s for one line-shape fit.

Computer Physics Communications 23 (1981) 411–426
North-Holland Publishing Company

# FORTRAN PROGRAM SPALL FOR COMPUTING SPALLATION REACTION CROSS SECTIONS

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Received 13 February 1981

## PROGRAM SUMMARY

*Title of program*: SPALL

*Catalogue number*: AAVE

*Computer*: UNIVAC 1108; *Installation*: Helsinki University of Technology, Helsinki, Finland

*Operating system*: EXEC8

*Programming language used*: FORTRAN IV

*High speed store required*: 16 000 words

*Number of bits in a word*: 36

*Overlay structure*: none

*Number of magnetic tapes*: none

*Other peripherals used*: card reader and line printer

*Number of cards in combined program and test deck*: 1247

*Keywords*: spallation reactions, cross sections, Rudstam formulae, Silberberg–Tsao formulae

*Nature of the physical problem*
Spallation reactions take place when high-energy hadrons (protons, neutrons or pions) collide with nuclei. The emission of a large number of nucleons is possible in these reactions leading to a large variety of product nuclides, many of which are radioactive.
The program SPALL is designed to compute spallation yield cross sections for different products from various targets as a function of the incident hadron energy.

*Method of solution*
The spallation yield cross sections are computed according to semiempirical formulae published by Rudstam and Silberberg and Tsao.

*Restrictions on the complexity of the problem*
The semiempirical formulae can be best applied to medium heavy and heavy nonfissionable target nuclides, which have also been used in the parameter fitting. The formulae should not be used when the difference in target and product masses is very large or very small. The incident hadron energy is usually tens of MeV or more. No difference is made between incident hadrons of different types, but the formulae are based mainly on data from proton irradiations.

*Typical running time*
On the UNIVAC 1108 computer the typical running time for a single reaction product at 40 energy points is about 0.35 s of CPU time.

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Computer Physics Communications 23 (1981) 427–433
North-Holland Publishing Company

# ORTHOGONALIZATION OF DISCRETE COORDINATES

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Received 28 May 1981

## PROGRAM SUMMARY

*Title of program*: RECT

*Catalogue number*: AAQW

*Computer*: CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: SCOPE 2.1.5

*Programming language used*: FORTRAN IV

*High speed storage required*: 13 200 words

*No. of bits in a word*: 60

*Overlay structure*: none

*Other peripherals used*: line printer, card reader

*No. of cards in combined program and test deck*: 542

*Keywords*: general purpose, orthogonalization, discrete orthogonal coordinates, boundary fitted coordinates, waterbag methods

*Nature of physical problem*
A two-dimensional boundary fitted orthogonal coordinate mesh may be required initially in an Eulerian calculation or at each time step in a semi-Lagrangian or waterbag [1] code. A procedure for orthogonalizing a non-orthogonal coordinate mesh is described which preserves one set of coordinates. The preserved coordinate lines may be open or closed.

*Method of solution*
The procedure is based upon an initial-value formulation [2] with the non-orthogonal coordinates as the independent variable. The initial-value problem is solved in its partial differential equation form.

*Restrictions on the complexity of the problem*
The initial non-orthogonal mesh must be smooth.

*Typical running time*
The running time scales linearly with the number of mesh points. On a CDC 7600 RECTC requires 0.037 s per 1000 points and RECTO requires 0.016 s per 1000 points.

*References*

[1] D.E. Potter, in: Methods in computational physics, vol. 16, eds. B. Alder, S. Fernbach and M. Rotenburg (Academic Press, New York, 1970) p. 43.
[2] C.W. Davies, J. Comput. Phys. 39 (1981) 164.

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North-Holland Publishing Company

# SAMPO80: MINICOMPUTER PROGRAM FOR GAMMA SPECTRUM ANALYSIS WITH NUCLIDE IDENTIFICATION

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Received 2 March 1981

## PROGRAM SUMMARY

*Title of program*: SAMPO80

*Catalogue number*: ABQO

*Computer for which the program is designed and others upon which it is operable*: DGC Nova and Eclipse line computers

*Computer*: Nova 2; *Installation*: Helsinki University of Technology, Finland

*Operating system*: RDOS

*High speed store required*: <25 kwords

*Number of bits in a word*: 16

*Programs overlaid*: yes

*Number of magnetic tapes*: none

*Other peripherals used*: console and line printer

*Number of lines in combined program and test deck*: 3000

*Keywords*: gamma spectroscopy, activation analysis, least squares fitting, nuclide identification

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Computer Physics Communications 24 (1981) 37–61
North-Holland Publishing Company

# FPPAC: A TWO-DIMENSIONAL MULTISPECIES NONLINEAR FOKKER–PLANCK PACKAGE

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Received 24 April 1981

## PROGRAM SUMMARY

*Title of program*: FPPAC

*Catalogue number*: AAQU (CRAY version), AAQV (CDC version)

*Computer*: CRAY-1, CDC-7600; *Installation*: National Magnetic Fusion Energy Computer Center, Lawrence Livermore National Laboratory

*Operating system*: CTSS on CRAY, LTSS on 7600

*Programming language used*: FORTRAN (ANSI 77), except for names exceeding 6 characters in length

*High speed storage required*: 304000B words (for mesh size 71 ($v$) by 31 ($\theta$), 2 general species, 1 Maxwellian species, 9 Legendre polynomials)

*No. of bits in a word*: 64 (CRAY), 60 (7600)

*Overlay structure*: none

*No. of cards in combined program and test deck*: 7000 per machine

*Keywords*: two-dimensional, multispecies, implicit, nonlinear, Fokker–Planck

*Nature of the physical problem*
The complete nonlinear multispecies Fokker–Planck collision operator for a plasma in two-dimensional velocity space is solved. The operator is expressed in terms of spherical coordinates ($v$ = speed, $\theta$ = angle between velocity and magnetic field directions, $\phi$ = azimuthal angle) under the assumption of azimuthal symmetry. Provision is made for additional physics contributions.

*Method of solution*
The Fokker–Planck equation is solved using finite differences. Spatial derivatives are approximated by central differences. Time-advancement is accomplished through either implicit operator splitting, an alternating direction implicit (ADI) algorithm, or fully implicit differencing. (In the latter case the user must supply his own nine-banded linear systems solver.) The Fokker–Planck coefficients and their derivatives are computed by expanding the distribution functions and the Rosenbluth potentials [1] in Legendre series, and equating the respective series coefficients.

*Restrictions on the complexity of the problem*
The user must adjust the number of meshpoints in the two coordinate directions as well as the number of Legendre polynomials used to calculate the Fokker–Planck coefficients. Sufficient accuracy for most problems is attained on both the CRAY and 7600. However, double precision should be used on a 32-bit-word machine.

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[*] Work performed under the auspices of the U.S.D.O.E. by Lawrence Livermore National Laboratory under contract W-7405-ENG-48.

*References*

[1] J. Killeen, A.A. Mirin and M.E. Rensink, in: Methods in computational physics, vol. 16 (Academic Press, New York, London. 1976) p. 389.
[2] J. Killeen and A.A. Mirin, in: College in theoretical and computational plasma physics, Trieste, 1977 (IAEA, Vienna, 1977) p. 27.
[3] M.G. McCoy, A.A. Mirin and J. Killeen, Scientific Computer Exchange Meeting, Livermore (1979) UCRL-83206.
[4] A.I. Shestakov, Lawrence Livermore Laboratory Internal Document UCID-18560 (1980).

*Note*: Separate source decks for CRAY-1 and CDC-7600 versions are provided.

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North-Holland Publishing Company

# SIMULATION OF PHOTOGRAPHIC IMAGES ON A PLOTTER

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Received 1 December 1980

## PROGRAM SUMMARY

*Title of program*: PHOTO SIMULATION

*Catalogue number*: AAQG

*Computer*: IBM 370/138, 370/168

*Operating system*: OS

*Programming language used*: FORTRAN IV

*High speed storage required*: 1612 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: one if display is on an off-line CALCOMP PLOTTER 936, none if display is on a VIDEO TEKTRONIX 4010/4014

*Other peripherals used*: line printer, card reader

*No. of cards in combined program and test deck*: 397

*Keywords*: simulation, photo, visualization of numerical array

*Nature of physical problem*
The subroutine may be usefully applied to visualize the output intensity of a function of two variables (in either Cartesian or polar coordinates), and/or follow its time evolution; example of application: mapping, stresses picture simulation, etc.

*Method of solution*
A coordinate grid is defined for the two independent variabl and each cell thus defined is filled with points randomly scattered within the cell, the density of plotting being propo tional to the average of the four values of the intensity at the four corners of the cell.

*Typical running time*
Per $dm^2$ of plot at a print density of 20 dots per $cm^2$ the running time is 50 s on an IBM 370/138 and 4.1 s on an IBM 370/168.

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* CNEN fellow.

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# A MONTE CARLO PROGRAM FOR QCD EVENT SIMULATION IN ELECTRON–POSITRON ANNIHILATION AT LEP ENERGIES

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Received 6 March 1981

## PROGRAM SUMMARY

*Title of program*: MULTJ

*Catalogue number*: AAVF

*Computer*: CDC 7600; *Installation*: CINECA, Bologna; the program has also been run at CERN, Geneva

*Operating system*: Scope 2.1.5 and NOS/BE

*Programming language used*: FORTRAN IV, extended

*High speed storage required*: 106 472B words – can be varied according to the choice of parameters

*No. of bits in a word*: 60

*Overlay structure*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 1923

*Keywords*: Monte Carlo generation, event simulation, quantum chromodynamics, electron–positron annihilation, multi-emission of quanta, leading-logarithm approximation

*Nature of physical problem*
Event simulation of quantum chromodynamics in the process electron + positron → virtual photon → hadrons at moderate and very high energies, assuming the leading logarithm approximation and including the multiemission of QCD quanta.

*Method of solution*
Monte Carlo generation of emitted QCD quanta by a procedure developed in ref. [1].

*Restrictions on the complexity of the problem*
Applications at low energy are limited to c.m.s. energies above 5–6 GeV, because of the physical approximations involved. At very high energy one may meet limitations associated with storage requirements.

*Typical running time*
At a c.m.s. energy of 40 GeV, 0.02 s per event on average

*Unusual features of the program*
A random number generating routine should be added. The sample driving program requires the addition of externals, as specified.

*References*

[1] R. Odorico, Nucl. Phys. B172 (1980) 157.

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Computer Physics Communications 24 (1981) 89–95
North-Holland Publishing Company

# TWO SUBROUTINES FOR CALCULATING LATTICE SUMS AND THE DISTORTION FIELD DUE TO A POINT FORCE IN HEXAGONAL SYSTEMS

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Received 4 May 1979; in revised form 22 May 1981

## PROGRAM SUMMARY

*Title of program*: HEXALAT

*Catalogue number*: QCKQ

*Computer*: Honeywell Bull 66/80 DPS; *Installation*: MPI Stuttgart

*Operating system*: GCOS

*Programming language used*: FORTRAN

*High speed store required*: 23 kwords

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 445

*Keywords*: solid state physics, hexagonal systems, elasticity theory, continuum Green's function, lattice sums, location and diffusion of interstitials

*Nature of physical problem*
In solid state theory the calculation of lattice sums in a perfect as well as in a distorted lattice is frequently required. HEXALAT contains two subroutines which can be used for calculations of this kind in the case of hexagonal systems. The subroutine ARRANGE generates the coordinates of a roughly spherical arrangement of atoms occupying the regular sites of an hcp structure. The coordinates are all stored in one array and can be used for calculating lattice sums. The subroutine DISPL calculates the displacement of an atom due to a double force tensor centered at the origin of the coordinate system in the elastic approximation. As an example, HEXALAT calculates the potential energy of an interstitial at an octahedral site both in the undistorted and in the distorted hexagonal lattice. The interaction potential between the interstitial and one atom is assumed to be given. Calculations of this kind are essential for the determination of the most stable sites for an interstitial and for the investigation of the diffusive behaviour.

*Method of solution*
The procedure used by ARRANGE is elementary and described in detail in the long write-up. DISPL uses the analytic expressions for the derivatives of the continuum Green's function. The parameters needed by DISPL depend on the elastic constants and are supplied by the subroutine PARA.

*Restrictions on the complexity of the problem*
HEXALAT is written in single precision. DISPL is restricted to the evaluation of displacements due to a diagonal double force tensor $P$ with $P_{11} = P_{22}$ (which holds for point defects at usual interstitial sites).

*Typical running time*
The execution time depends on the number of atoms in the arrangement. The test run (180 atoms) on the Honeywell Bull 66/80 DPS took 2.1 s for compilation and 2.0 s for execution.

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North-Holland Publishing Company

# BESSEL FUNCTIONS $I_\nu(z)$ AND $K_\nu(z)$ OF REAL ORDER AND COMPLEX ARGUMENT

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Received 17 June 1981

## PROGRAM SUMMARY

*Title of program*: BESSIK

*Catalogue number*: AAQZ

*Computer*: IBM 3033; *Installation*: National Research Council, Ottawa

*Operating system*: TSS/370

*Programming language used*: FORTRAN IV

*High speed storage required*: 14700 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1955

*Keywords*: general purpose, Bessel, cylindrical, backward recurrence, Miller's algorithm, complex functions

*Nature of the physical problem*
Bessel functions appear in a large number of physical problems, e.g., the solution of potential problems in cylindrical coordinates.

*Method of solution*
For arguments of small or moderately large modulus, $I_\nu(z)$ is computed by Miller's backward recurrence algorithm described by Gautschi [1]. For arguments of large modulus, $I_\nu(z)$ is determined from its asymptotic expansion for large argument and backward recurrence.

$K_\nu(z)$ and $K_{\nu+1}(z)$ for $|\nu| \leqslant 1/2$ are determined from Neumann series when real part of $z$ is small [2] and from Temme's algorithm [3] and some modifications [4] for arguments of moderately large or large modulus. For real arguments, Temme's algorithm for small arguments is also used. $K_\nu(z)$ for large order is obtained from the forward recurrence.

*Restrictions on the complexity of the problem*
The functions are determined only for non-negative order. $K_\nu(z)$ is determined only for values of $z$ with non-negative real part. The subroutines are inefficient when both order and modulus of argument are very large.

*Typical running time*
For order and modulus of argument not both large, the determination of a single function requires less than 1.6 ms. The determination of a sequence of functions with the orders of two successive members of the sequence differing by 1 requires, in addition, 15 $\mu$s for each member of the sequence. The running times of subroutines RBESI and RBESK for real argument are comparable to those of RBESJ and RBESY [5] and are about 1/2 to 1/3 of the running times of subroutines CBESI and CBESK for complex argument. Running times on the IBM 3033 are about 1.9 times faster than times on the IBM 3032 which was the computer used for the results reported in ref. [5].

*Accuracy*
The subroutines are written in double precision arithmetic for real argument and in double precision complex arithmetic for complex argument. The accuracy obtained is approximately 14 digits except when $z$ is close to a zero of the function.

*References*

[1] W. Gautschi, SIAM Rev. 9 (1967) 24.

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[2] M. Goldstein and R.M. Thaler, Math. Tables Aids Comput. 13 (1959) 102.
[3] N.M. Temme, J. Comput. Phys. 19 (1975) 324.
[4] J.B. Campbell, ACM Trans. Math. Software 6 (1980) 5
[5] J.B. Campbell, Comput. Phys. Commun. 18 (1979) 13

Computer Physics Communications 24 (1981) 113–125
North-Holland Publishing Company

# A FLEXIBLE PROGRAM FOR PERFORMING ANALYTIC DIFFERENTIATION AND SUBSTITUTIONS ON A SYSTEM OF EQUATIONS

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Received 5 May 1981

## PROGRAM SUMMARY

*Title of program*: EQSYSTM

*Catalogue number*: AAQX

*Computer*: IBM 370/3033; *Installation*: Pennsylvania State University Computation Center, University Park, PA 16802, USA

*Other computers on which operable*: any IBM Series 360/370 computer, and any non-IBM computer with IBM 360/370-compatible architecture

*Operating system*: MVS

*Programming language used*: PL/1-FORMAC 73 [1]

*High speed storage required*: storage is dynamically allocated and released by the program as needed, depending on the input data deck. The minimum available on the Penn. State system – 300 Kbytes – usually proves sufficient

*No. of bits in a word*: 32

*Overlay structure*: none required; however, the program consists of a main program that calls three subroutines in succession, making feasible a simple overlay structure. This is included along with the program deck

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, card punch, disk

*No. of cards in combined program and test deck*: 1986

*Keywords*: (symbolic) algebraic language, Jacobian matrix, nonlinear equations, nonlinear regression, (symbolic) differentiation, (partial) derivative(s), (symbolic) substitution, FORMAC, PL/1, PL/C, FORTRAN, SAS, MINPACK

*Nature of physical problem*
This program is designed to operate on a system of equations, making user-specified substitutions and returning for each expression its partial derivatives with respect to a list of specified variables. The output expressions for the derivatives of each input expression, in the form of statements directly usable in other programs, are organized into an array with subscripts corresponding to the variables by which it was differentiated. Output in either PL/1 [2], FORTRAN or SAS [3] syntax is available at user option.

*Method of solution*
The program makes use of the powerful symbolic algebraic manipulation facilities of the PL/1-FORMAC73 language.

*Restrictions on the complexity of the problem*
The maximum length of input expressions depends only on the limits inherent in the PL/1 compiler itself (32 765 characters (ref. [2], p. 411) in the current IBM implementation of PL/1). Output expressions are normally limited to 5000 characters. There are no a priori limits on the number of variables, substitutions or expressions to be differentiated; these are ultimately limited by installation resources and the FORMAC system itself, and are unlikely to be exceeded by most users. The program can be used to determine derivatives beyond first order, up to a maximum of fourth order.

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* Daniel W. Merdes was an employee of the Pennsylvania State University Computation Center for a portion of the time that he worked on this program.

*References*

[1] K.A. Bahr, FORMAC73 user's manual (IBM-SHARE Program #360D-03.3.013, SHARE Program Library Agency, Triangle Universities Computation Center, Research Triangle Park, NC 27709, USA).

[2] OS PL/1 checkout and optimizing compilers: language reference manual (IBM Program Product GC33-0009-4, File No. S360/S370-29, International Business Machines Corp., 1976).

[3] SAS user's guide, 1979 edition (SAS Institute, Inc., P.O. Box 10066, Raleigh, NC 27605, USA, 1979).

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North-Holland Publishing Company

# MONTE CARLO SIMULATION OF SU(2) LATTICE GAUGE THEORY

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Received 1 June 1981

## PROGRAM SUMMARY

*Title of program*: SU2LGT

*Catalogue number*: AAQY

*Computer*: CDC 6600, CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: CDC NOS/BE, SCOPE

*Programming language used*: FORTRAN IV

*High speed storage required*: 18 K (maximum)

*Number of bits in a word*: 60

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 724

*Keywords*: lattice gauge theory, SU(2) gauge theory, Yang–Mills theory, non-Abelian gauge theory, non-perturbative effects, phase transitions, statistical mechanics, action per plaquette, Monte Carlo Techniques

*Nature of the physical problem*
The program calculates the average action per plaquette for SU(2) lattice gauge theory. Gauge theories on a lattice were originally proposed by Wilson [1] and Polyakov [2]. This paper is largely based on the method adopted by Creutz [3] for the Monte Carlo study of SU(2) gauge theory.

*Method of solution*
A Monte Carlo simulation of the system set up on a lattice (with varying numbers of sites per dimension considered) under an SU(2) gauge field, generates a series of field configurations. The heat bath method of ref. [4] is used to produce statistical equilibrium, and a hot and cold (disordered and ordered) start can be used to determine when statistical equilibrium is achieved.

*Restrictions on the complexity of the program*
The storage required is dependent on the number $N$ of dimensions and the number $L$ of lattice sites along each dimension. The arrays in the program that usually have the largest dimensions are dimensioned to $N(L)^N$ (i.e. the number of links involved in the lattice). The execution time increases with the number of links and the number of Monte Carlo iterations.

*Typical running time*
The test run with a 4-dimensional lattice of 4 sites per dimension and 60 Monte Carlo iterations took 45 s for execution on the CDC 6600 at ULCC.

*References*

[1] K.G. Wilson, Phys. Rev. D10 (1974) 2455.
[2] A.M. Polyakov, unpublished.
[3] M. Creutz, Phys. Rev. D21 (1980) 2308.
[4] M. Creutz, L. Jacobs and C. Rebbi, Phys. Rev. D20 (1979) 1915.
K. Binder, in: Phase transitions and critical phenomena, vol. 5B, eds. C. Domb and M.S. Green (Academic Press, New York, 1976).

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Computer Physics Communications 24 (1981) 135–140
North-Holland Publishing Company

# GENERATION OF SYMMETRY-ADAPTED FUNCTIONS FOR MOLECULAR CALCULATIONS

Lubomír SKÁLA
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Received 7 June 1981

## PROGRAM SUMMARY

*Title of program*: SYMMET

*Catalogue number*: AAPD

*Computer*: ICL 4-72; *Installation*: University Regional Computing Centre, Prague

*Computer on which it is operable*: IBM 360/370 (FORTRAN H compiler)

*Operating system*: MULTIJOB

*Programming language used*: FORTRAN (IBM version)

*High speed storage required*: 2208 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer

*No. of cards in combined program and test deck*: 1254

*Keywords*: electronic structure, molecule, symmetry-adapted function, point group, irreducible representation

*Nature of physical problem*
The group theory is used for the classification of energy states of molecules and the transformation of the eigenvalue problem to a quasidiagonal form.

*Method of solution*
Symmetry-adapted linear combinations of the basis functions and other information are obtained by means of the symmetrizing operator.

*Restrictions on the complexity of the problem*
All the most important point groups are included. There is no restriction on the number of the basis functions.

*Typical running time*
The running time is usually negligible in comparison with other steps of the electronic structure calculation. The test run took 30 s on an ICL 4-72.

Computer Physics Communications 24 (1981) 141–159
North-Holland Publishing Company

# KLEIN: COULOMB FUNCTIONS FOR REAL λ AND POSITIVE ENERGY TO HIGH ACCURACY

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*Department of Physics, Schuster Laboratory, University of Manchester, Manchester, M13 9PL, UK*

Received 1 June 1981

## PROGRAM SUMMARY

*Title of program*: KLEIN: Coulomb WFN, Real L, ETA, X

*Catalogue number*: ABNJ

*Computer*: IBM 370/165 and AS/7000; *Installation*: Daresbury Laboratory, Warrington, Lancs.

*Operating system*: OS/360 G1 compiler and HX compiler (level 2.2.1)

*Programming language used*: ASA FORTRAN

*High speed storage required*: 46 kbytes ≈12 kwords

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, printer

*No. of cards in combined program and test deck*: 316

*Keywords*: Klein–Gordon, Coulomb for real angular momentum, Dirac, Schrödinger, Bessel, spherical Bessel, continued-fraction, reactions, scattering, heavy-ion, nuclear, molecular, atomic, pionic, kaonic, exotic atoms, scattering states, *N*-dimensional H-atom

*Nature of the physical problem*
KLEIN computes relativistic Schrödinger (Klein–Gordon) equation solutions, i.e. Coulomb functions for real $\lambda > -1$, $F_\lambda(\eta, x)$, $G_\lambda(\eta, x)$, $F'_\lambda(\eta, x)$ and $G'_\lambda(\eta, x)$ for real $x > 0$ and real $\eta$, $-10^4 \leqslant \eta \leqslant 10^4$. Hence it is also suitable for Bessel and spherical Bessel functions. Accuracies are in the range $10^{-14}$–$10^{-16}$ in oscillating region, and $\approx 10^{-30}$ on an extended precision compiler. The program is suitable for generating Klein–Gordon wavefunctions for matching in pion and kaon physics.

*Method of solution*
An extended version of Steed's method used previously for integer λ in subroutine RCWFN [1], is adopted.

*Restriction on the complexity of the problem*
The standard version loses accuracy as $x < x_\lambda$ (the turning point) and eventually when $G \gtrsim 10^6$ the subroutine is ineffective; a JWKB approximation and full information is output.

*Typical running time*
The test deck took about 2 s to run on the G1 compiler, and HX compiler; with AUTODBLE and REAL*16 variables the same deck took 76 s (ACCUR = $10^{-16}$) and 109 s (ACCUR = $10^{-33}$). Note that about one half the time demonstrates error conditions.

*Reference*
[1] A.R. Barnett, D.H. Feng, J.W. Steed and L.J.B. Goldfarb, Comput. Phys. Commun. 8 (1974) 377.

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Computer Physics Communications 24 (1981) 161–172
North-Holland Publishing Company

# A PROGRAM FOR CALCULATION OF THE CORIOLIS EFFECT IN ODD–ODD NUCLEI

Z. HONS
*Laboratory of Nuclear Problems, Joint Institut for Nuclear Research, Dubna, USSR*

and

J. KVASIL
*Laboratory of Theoretical Physics, Joint Institute for Nuclear research, Dubna, USSR*

Received 19 June 1981

## PROGRAM SUMMARY

*Title of program*: ODDODDCORI

*Catalogue number*: AARA

*Computer*: CDC 6500; *Installation*: Laboratory of Calculating Techniques and Automation, Joint Institute for Nuclear Research, Dubna, USSR

*Operating system*: NOS/BE 1

*Programming language used*: FORTRAN

*High speed storage required*: 32100 words (MINUIT included)

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1204

*CPC library subprogram used*:

*Catalogue number*: ACWH; *Title*: MINUIT; *Ref. in CPC*: 10 (1975) 343

*Keywords*: nuclear, Coriolis effect, fitting, experimental, energy level, deformed nuclei, odd–odd nuclei

*Nature of physical problem*
Many papers have been devoted recently to particle-rotational coupling (Coriolis effect) in odd deformed nuclei (e.g. refs. [1–4]), when the experimental spectrum could be often explained by this coupling. Therefore, one can expect that the Coriolis coupling plays, as well, a significant role in odd–odd deformed nuclei for which a lot of experimental data appeared lately (e.g. ref. [5]). The program makes it possible to extract pure intrinsic energy values from experimental data. This is important for testing the theoretical models for intrinsic structure of odd–odd nuclei. The program calculates the perturbed energy levels. It is written as a subroutine to be used with the MINUIT minimization program [6], which makes a least-square fit to the experimental energy levels. Mixed amplitudes of the wave functions are obtained for the final fit.

*Method of solution*
In order to take the Coriolis coupling into account, the matrix of the total Hamiltonian is constructed and diagonalized. The Jacobi diagonalization method is used repeatedly in the search for eigen values and coupling and amplitudes for all spin values. Simultaneously, the adjustment of all the parameters is carried out untill a least-square fit to the experimental energy levels is obtained.

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*References*

1] G. Løvhøiden and I. Kanestrøm, Phys. Norv. 6 (1972) 33.

2] G. Løvhøiden, P.O. Tjøm and L.O. Edvarson, Nucl. Phys. A194 (1972) 463.

[3] S.A. Hjorth, A. Johnson and G. Ehrling, Nucl. Phys. A184 (1972) 113.

[4] P. Hornshøj, P. Tidemand-Petersson, R. Kaczarowski, B. Kotlinska and J. Zylicz, Nucl. Phys. A248 (1975) 406.

[5] C.M. Lederer and V.S. Shirley, Table of isotopes, Seventh ed. (1978).

[6] F. James and M. Roos, Comput. Phys. Commun. 10 (1975) 343.

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Computer Physics Communications 24 (1981) 173–179
North-Holland Publishing Company

# TETRAHEDRAL FINITE ELEMENT MATRIX PRIMITIVES

Peter P. SILVESTER, F.U. MINHAS and Z.J. CSENDES
*Electrical Engineering Department, McGill University, Montreal H3A 2A7, Canada*

Received 16 April 1981

## PROGRAM SUMMARY

*Title of program*: TETRAHEDRAL MATRIX PRIMITIVES

*Catalogue number*: AARB

*Computer*: Any PDP-11 for demonstration; any machine with ANSI Fortran compiler for subroutine package

*Operating system*: Demonstration programs run under RT-11 system. Subroutine package is system-independent

*Programming language*: Fortran IV

*High speed storage required*: approx. 25 Kwords

*No. of bits in a word*: 16 for demonstration programs. Subroutine package resets itself at run-time to the necessary precision level

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: none for subroutine package. Standard interactive terminal (VDU) for demonstration programs.

*No. of cards in combined program and test deck*: 930

*Keywords*: finite elements, matrix primitives, tetrahedral elements, three-dimensional analysis, boundary value problems, primitive matrices, universal matrices

*Nature of physical problem*
TETRAHEDRAL MATRIX PRIMITIVES is a subroutine package for constructing finite element representations of arbitrary linear second-order differential operators. Finite element matrices for any such operator may be constructed from three matrix primitives. The results are of use in three-dimensional potential and flow problems, electromagnetics of plasmas, diffusion problems and elsewhere.

*Method of solution*
The primitives are constructed for any specified order $N$ of polynomial approximation, by computing the standard tetrahedron interpolation polynomials, then differentiating and integrating them as required. Differentiations are performed analytically, while integrations use Newton–Cotes quadrature of sufficiently high order to guarantee zero discretization error. The precision level attainable on the machine used is checked by the program at run-time.

*Restrictions on the complexity of the problem*
Matrices for interpolation orders beyond 7 or 8 may suffer from round-off error accumulation.

*Typical running time*
On PDP-11/03 with KEV-11, about two hours for matrices of order 4. On IBM 370/165, about 8 min.

*Unusual features of the program*
The available machine precision is determined by the program itself at run-time.

*References*
A full theory of tetrahedral finite element generation is given in:
P.P. Silvester, Intern. J. Num. Meth. Eng. (1981) in press.

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Computer Physics Communications 24 (1981) 181–184
North-Holland Publishing Company

# BAND STRUCTURE CALCULATIONS OF CUBIC SEMICONDUCTORS ON THE BASIS OF LÖWDIN'S PERTURBATION TECHNIQUE

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*Laboratory for Theoretical Physics, Boris Kidrič Institute for Nuclear Sciences, Belgrade, Yugoslavia*

Received 10 June 1981

## PROGRAM SUMMARY

*Title of program*: EBCLP

*Catalogue number*: AARC

*Computer*: CDC-3600; *Installation*: Boris Kidrič Institute of Nuclear Sciences, Beograd

*Operating system*: SCOPE 6, 3

*Programming language used*: FORTRAN

*High speed storage required*: 35046 words

*No. of bits in a word*: 48

*Overlay structure*: none

*Other peripherals used*: CR

*No. of cards in combined program and test deck*: 358

*CPC library subprograms used*: RECIPS

*Keywords*: **k**-space, energy bands, solid state physics

*Nature of physical problem*
This work is concerned with the band structure calculations of cubic semiconductors.

*Method of solution*
We applied Brust's modification of Löwdin's perturbation technique [1] for the energy band calculations of the cubic semiconductors. With this technique the band structure calculation problem reduces to the eigenvalue problem of the truncated complex symmetrical matrix.

*Restrictions on the complexity of the problem*
Only for cubic semiconductors

*Typical running time*
For two points in **k**-space this program needs about 3 min.

*Reference*

[1] D. Brust, Phys. Rev. 134 (1964) A1337.

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Computer Physics Communications 24 (1981) 185–190
North-Holland Publishing Company

# RECURRENCE SOLUTION OF A BLOCK TRIDIAGONAL MATRIX EQUATION WITH NEUMANN, DIRICHLET, MIXED OR PERIODIC BOUNDARY CONDITIONS

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*Department of Physics, Imperial College of Science and Technology, London SW7 2BZ, UK*

Received 23 July 1981

## PROGRAM SUMMARY

*Title of program*: PERDIAG

*Catalogue number*: AARF

*Computer*: CDC 6500; *Installation*: Imperial College Computer Centre

*Operating system*: NOS

*Programming language used*: FORTRAN IV

*High speed storage required*: 17.7 Kwords

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 445

*Key words*: matrix equation, perdiagonal, tridiagonal, $n \times n$ blocks, direct method, recursive, periodic boundary conditions, $n$ finite difference equations, one space dimension, implicit

*Nature of physical problem*
A theorist may wish to solve the matrix equation $AU = W$, rapidly, where $A$ is a block tridiagonal matrix. This type of matrix equation frequently arises in the solution of problems in one space dimension; in the solution of boundary-value and many initial-value problems (because the time-dependent problem has been formulated implicitly), where it is necessary to solve $n$ coupled, finite difference equations. The program is capable of dealing with Neumann, Dirichlet, mixed or periodic boundary conditions. If the boundary conditions are periodic, the resulting matrix $A$ is block tridiagonal with additional blocks in the upper right and left corners, referred to here as block perdiagonal.

*Method of solution*
A recurrence solution is used to solve the matrix equation $AU = W$. The method follows the principles for a recurrence solution of a tridiagonal matrix equation [1], modified, when appropriate, to deal with the more complex case of periodic boundary conditions.

*Restrictions on the complexity of the problem*
None. The method does not assume any particular properties of the $n \times n$ submatrices, other than their being non-singular.

*Typical running time*
The test runs took about 0.3 s. Generally, the running time would depend on the size of the blocks and the number of mesh points.

*References*

[1] D. Potter, Computational physics (John Wiley, London, 1972).

Computer Physics Communications 24 (1981) 191–196
North-Holland Publishing Company

# GENERATING FUNCTIONS FOR $L$-HARMONICS

R.W. GASKELL
*Department of Physics, Lafayette College, Easton, PA 18042, USA*

Received 3 August 1981

## PROGRAM SUMMARY

*Title of program*: LHARM

*Catalogue number*: AARE

*Computer*: HP 3000; *Installation*: Lafayette College, Easton, PA, USA

*Operating system*: MPEIII

*Programming language used*: FORTRAN

*High speed storage required*: 25440 words

*No. of bits in a word*: 16

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: disc drive, terminal

*No. of lines in program*: 137 (including comment statements)

*Keywords*: $L$-harmonics, generating function, generalized SU(2) spherical harmonics, SU(2), O(3), Lie group, Lie algebra

*Nature of physical problem*
Generating functions enumerating $L$-harmonics are useful in providing polynomial bases and constructing missing label operators for semisimple groups reduced according to the principal SU(2) subgroup. LHARM can be used to construct such generating functions for arbitrarily large $L$.

*Method of solution*
Recursion procedure generating $F_L$ from $F_{L-2}$.

*Restrictions on the complexity of the problem*
There are no restrictions but some modifications are needed in the listed program for $L > 13$.

*Typical running time*
Compile time was 3 s. For $L = 5$, CPU = 7. For $L = 13$, CPU = 72.

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Computer Physics Communications 24 (1981) 197–203
North-Holland Publishing Company

# INITIAL VALUES OF PARAMETERS FOR VARIABLE MOMENT OF INERTIA MODELS

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*Nuclear Research Center "Demokritos", Aghia Paraskevi-Attiki, Athens, Greece*

Received 12 October 1980; in final form 6 August 1981

## PROGRAM SUMMARY

*Title of program*: INVAP

*Catalogue number*: ABQN

*Computer*: CDC 3300; *Installation*: N.R.C. "Demokritos", Aghia Paraskevi-Attiki, Athens, Greece

*Operating system*: MASTER 4.1

*Program language used*: FORTRAN ANSI

*High speed storage required*: 20480 words

*No. of bits in a word*: 24

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 760

*Keywords*: nuclear, rotational spectra, spectroscopy, collective models, variable moment of inertia models, fitting

*Nature of physical problem*

The long write-up summarizes the procedure for determining the initial values of parameters for the fitting of rotational spectra in even–even nuclei. The functional form of the fitting is:

$$E_I = C_2(J_I - J_0)^2 + C_3(J_I - J_0)^3 + C_4(J_I - J_0)^4 + \dots$$

with the condition

$$\partial E_I / \partial J_I = 0,$$

where $E_I$ and $J_I$ are the excitation energy and moment of inertia at a certain angular momentum $I$, respectively, and $C_i$ and $J_0$ are the parameters of interest. While the determination of these parameters can be done following several standard fitting procedures, in all cases (since we always have to solve a nonlinear system of equations), there is a great sensitivity to the initial values of these parameters. The purpose of this paper is to determine initial values suitable for any standard fitting procedure, by using an approximate solution of the problem.

omputer Physics Communications 24 (1981) 205–223
orth-Holland Publishing Company

# A TIME-OF-FLIGHT SPECTRUM SIMULATOR FOR NEUTRON ELASTIC AND INELASTIC SCATTERING

Gunter H.R. KEGEL
*Physics Department, University of Lowell, Lowell, MA 01854, USA*

Received 13 May 1981

## PROGRAM SUMMARY

*itle of program*: IMBUI-G, NEUTRON TOF SIMULATOR

*atalogue number*: ABKJ

*omputer*: HP1000; *Installation*: University of Lowell

*perating system*: RTE-II

*rogramming language used*: Assembler language

*igh speed storage required*: 12000 words

*o. of bits in a word*: 16 (fixed point), 32 (floating point)

*eripherals used*: disc, printer

*o. of records in combined program and test deck*: 2225

*ey words*: neutron, cross section, time-of-flight spectrum, mulation, scattering, numerical integration, disc scatterer

*ature of physical problem*
ogram IMBUI was written to assist in the design and the ta analysis of high resolution ($\Delta E/E \approx 1\%$) neutron time--flight experiments using a subnanosecond, pulsed Van-de-Graaff accelerator. Several factors govern the resolution in these experiments; there are timing uncertainties, variations in neutron velocities, and uncertainties in flight path lengths. Through careful selection of experiment parameters it is possible to optimize resolution without sacrificing the detector counting rate. IMBUI assists in this task by providing the user with simulated time spectra, which include geometric and kinematic effects.

*Method of solution*
Time-of-flight spectra may be obtained as integral transforms involving integration over the scatterer volume. IMBUI evaluates these scatterer integrals using appropriate numerical techniques.

*Restrictions on the complexity of the problem*
The following effects are not taken into account:

1. Neutron multiple scattering. These contributions may be obtained from other codes.
2. Finite burst duration from the accelerator.
3. Finite electronic time resolution of the detector.
4. Finite thickness of the neutron target.

*Typical running time*
Six seconds plus 17 ms per scatterer volume element.

*Reference*
The programming language used is described in the "RTE Assembler Reference Manual", Part No. 92060-90005, Hewlett-Packard Company, 11000 Wolfe Road, Cupertino, CA 95014, USA.

Computer Physics Communications 25 (1982) 21–28
North-Holland Publishing Company

# A PROGRAM FOR THE PREDICTOR–CORRECTOR NUMEROV METHOD

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*Department of Physics, University of Windsor, Windsor, Canada N9B 3P4*

Received 14 September 1981

## PROGRAM SUMMARY

*Title of program*: PCNUM

*Catalogue number*: AARJ

*Computer*: IBM 370/3031; *Installation*: University of Windsor Computer Centre

*Operating system*: OSMVT under VM

*Programming language used*: FORTRAN IV

*High speed storage required*: 10 Kwords (for 8 channels)

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 829

*Keywords*: coupled second-order differential equations, nonlinear equations, predictor–corrector method, Numerov, scattering calculations

*Nature of the physical problem*
Matrix differential equations of the form

$$\mathbf{y}''(x) = \mathbf{F}[x, \mathbf{y}(x)], \tag{1}$$

are solved, including homogeneous equations such as arise in quantum scattering theory.

*Method of solution*
A predictor–corrector version of the Numerov method is applied [1]. Step size is adjusted to maintain a specified accuracy, and solutions to homogeneous differential equations can be stabilized by orthogonalization.

*Restrictions on the complexity of the problem*
The matrices $\mathbf{y}$ and $\mathbf{F}$ are assumed to be real matrices with dimensions not exceeding 8 × 8 (they are not necessarily square). These restrictions may be removed at the cost of additional storage by adding appropriate COMPLEX*16 type declarations on the one hand, and by increasing array dimensions on the other. Although $\mathbf{F}$ may be a nonlinear function of $\mathbf{y}$, it is assumed that the $j$th column of $\mathbf{F}$ depends only on components in the corresponding column of $\mathbf{y}$. As with other Numerov algorithms, the equations to be solved need to be written so that there are no first-order derivatives.

*Unusual features of the program*
The error monitored is the relative error in the local change of the independent variable, and this is compared with the specified error limit to determine whether to halve, maintain or double the step size. Unlike other predictor–corrector methods, no special starting procedure is required. Solutions to linear problems can be stabilized to ensure linear independence. The stabilization is accomplished by periodic orthogonalization of the columns of $\mathbf{y}$ with the frequency of application determined by the amount of change caused by the orthogonalization.

*Typical running time*
Test runs with 4 channels (4 × 4 matrices) requiring evaluation at about 2500 points and stabilization, took 6 s to compile and 20 s to run on the IBM 370/3031.

*References*

[1] W.E. Baylis and S.J. Peel, Comput. Phys. Commun. 25 (1982) 7.

Computer Physics Communications 25 (1982) 29–38
North-Holland Publishing Company

# AN ADAPTATION OF ACQI TO CALCULATE THE DATA FOR MSXALPHA PROGRAM

M. KLOBUKOWSKI *
*Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada*

Received 29 June 1981

## ADAPTATION SUMMARY

*Title of adaptation*: ADAPT HFS FOR MSXALPHA

*Adaptation number*: 0001

*Reference to original program*:
*Cat. number*: ACQI; *Title*: H.F.S. SELF-CONSISTENT FIELD; *Ref. in CPC*: 1 (1969) 216

*Author of original program*: J.-P. Desclaux

*Computer*: Amdahl 470/V7; *Installation*: University of Alberta, Edmonton, Canada

*Operating system*: MTS

*Programming language used in adapted program*: FORTRAN IV

*High-speed core required*: 75656 bytes

*Number of bits in a byte*: 8

*Peripherals used*: card reader, line printer, disk

*No. of cards required to effect adaptation (including directive ards)*: 254

*dditional keywords*: SCF X$\alpha$ scattered wave method

*Nature of physical problem*
The adaptation allows one to prepare the numerical atomic orbitals data to be used by the new version of the SCF X$\alpha$ scattered wave program MSXALPHA/II [1]. The output file produced by the present adaptation conforms to the data requirement of that program.

*Method of solution*
The Hartree–Fock–Slater calculations are carried out for all the unique atoms of the molecule to be treated later by the MSXALPHA/II program. The atomic results are next restored from work files and rearranged into a form suitable for input to the MSXALPHA/II program.

*Restrictions on the complexity of the problem*
Due to dimensions of some arrays in subroutine MSINPT a maximum of 10 unique atoms may be treated. However, this restriction may be easily removed by increasing the array dimensions.
Other restrictions (maximum number of orbitals per atom, maximum number of integration points) are the same as those in the original program ACQI [2].

*Typical running time*
The CPU time required to compile the modified program was 6.3 s (FORTRAN H compiler). It took 2.7 s of the CPU time to run the first test run, and 3.3 s to run the second test run.

*References*

[1] S. Katsuki, M. Klobukowski and P. Palting, Comput. Phys. Commun. 25 (1982) 39.
[2] J.-P. Desclaux, Comput. Phys. Commun. 1 (1969) 216.

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* On leave from the Institute of Chemistry, N. Copernicus University, Toruń, Poland; I.W. Killam Postdoctoral Fellow 1980–1981.

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Computer Physics Communications 25 (1982) 39–55
North-Holland Publishing Company

# A COMPACT PROGRAM OF THE SCF-X$\alpha$ SCATTERED WAVE METHOD: VERSION II

Shinichi KATSUKI *, Mariusz KLOBUKOWSKI ** and Pancracio PALTING ***
*Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada*

Received 29 June 1981

## PROGRAM SUMMARY

*Title of program*: MSXALPHA/II

*Catalogue number*: AARD

*Computer*: Amdahl 470/V7; *Installation*: University of Alberta, Edmonton, Alberta, Canada

*Operating system*: MTS

*Programming language used*: FORTRAN IV

*High speed core required*: 488 Kbytes

*Number of bits in a byte*: 8

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals required*: card reader, line printer, disk

*Number of cards in the combined program and test deck*: 7052

*CPC Library subprogram used*:

*Catalogue number*: ACQI; *Title*: ADAPT HFS FOR MSXALPHA; *Ref. in CPC*: 25 (1982) 29

*Reference to other published version of this program*:

*Catalogue number*: ACXN; *Title*: MSXALPHA; *Ref. in CPC*: 14 (1978) 13

*Keywords*: Quantum chemistry, symmetry, muffin-tin approximation, nonoverlapping spheres, X$\alpha$ approximation, initial atomic orbitals, ground state, transition state

*Nature of the physical problem*
The contribution offered here is a modified version of the MSX$\alpha$ program presented earlier [1] which has been extended to accomodate the handling of twenty-six symmetry point groups. Otherwise the program is the same in that it computes molecular orbitals and energy levels for the ground state and transition states using the muffin-tin and X$\alpha$ approximations for the potential energy in the case of non-overlapping contingent spheres [2–5].

*Method of solution*
The starting atomic orbitals generate the potential in the muffin-tin and X$\alpha$ approximations, once the physical space of the molecule is appropriately divided into regions of contiguous nonoverlapping spheres. The Runge–Kutta–Milne method is used to solve the radial Schrödinger equation in the spherical atomic regions and in the extramolecular region if the Watson sphere is present. Energy eigenvalues and eigenvectors are obtained by determining the zeros of the secular determinant with the aid of the Gaussian elimination procedure with complete pivoting. A special algorithm is used to distinguish zeros from poles. A perturbation technique is used to accelerate the search for and the determination of the zeros (energy eigenvalues) [6]. Normalization of the calculated eigenvectors is carried through according to the method of Ham and Segall [7]. The newly determined molecular orbitals are now employed to construct the poten-

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[*] On leave from College of General Education, Kyushu University, Ropponmatsu, Fukuoka, Japan.

[**] On leave from Institute of Chemistry, N. Copernicus University, Toruń, Poland; I.W. Killam Postdoctoral Fellow 1980–1981.

[***] On leave from Departamenta de Química, Universidad Autónoma Metropolitana-Iztapalapa, México 13, DF.

tial. Again eigenvalues and eigenvectors are determined. The process is repeated until self-consistency is achieved, i.e., until some predetermined criterion concerning the convergence of the eigenvalues is satisfied.

*Restriction on the complexity of the problem*
Only the spin-restricted case is handled. Moreover, the symmetry point groups which can be treated are: $C_2$, $C_3$, $C_4$, $C_6$, $D_2$, $D_3$, $D_4$, $D_6$, $C_{2v}$, $C_{3v}$, $C_{4v}$, $C_{6v}$, $C_{2h}$, $C_{3h}$, $C_{4h}$, $C_{6h}$, $D_{2h}$, $D_{3h}$, $D_{4h}$, $D_{6h}$, $D_{2d}$, $D_{3d}$, $D_{4d}$, $D_{6d}$, $T_d$ and $O_h$.

*Typical running time*
The compilation time (FORTRAN H compiler) was 50.1 s on an Amdahl 470/V7. The CPU time of the initial calculation (the first test case) was 23.2 s. It took 59.3 s of CPU time to complete the first three SCF iterations (the second test case).

*Unusual features of the program*
The starting atomic orbitals may be either numerical Hartree–Fock orbitals or analytical Hartree–Fock orbitals in an STO or GTO basis. Let us define an atomic "species" as a set of symmetry equivalent atoms, i.e., by applying the operations of the symmetry group in question to any one member of the set, the other members of the species are generated. The present version of the program automatically generates all the members of a species, their coordinates and spherical harmonic basis functions, once these quantities are specified for one member of the species along with the specification of the symmetry group in question. Furthermore, the entire set of partner functions situated on the central atom which span the invariant subspace of a given irreducible representation is generated for a given maximum value of the quantum number $l$. Calculations may be done piece-wise and restarts may be made from a given iteration. Core orbitals may be frozen during a calculation. Initially valence levels are found by a brute-force scanning of an energy range with a determined mesh size. In order to reduce the computation time, in the next iterations only the narrow energy ranges around the perturbationally predicted eigenvalues are scanned.

Although the program was not overlaid in the calculations reported here, the code was rewritten so as to facilitate an implementation of overlay features of an operating system.

The input requirements were changed so as to match the output of the modified Hartree–Fock–Slater program [8,9]. The HFS numerical AO's were used as the starting data in the calculations provided as the test cases.

*FORTRAN compatibility*
Since the program is written in IBM FORTRAN IV, the following features may render it incompatible with other FORTRAN compilers:

(1) in subroutine INPOTL, arrays COEFF and DZT are four-dimensional;
(2) apostrophes are used in FORMAT statements to define Hollerith strings in place of the standard field description nH;
(3) array element expressions which involve another array element are used, e.g. NDG(IRG3(I));
(4) IMPLICIT REAL*8 statement is used;
(5) characters & and # are used in column 6 for continuation lines;
(6) the ENTRY statement is used;
(7) T format code is used.

*References*

[1] S. Katsuki, P. Palting and S. Huzinaga, Comput. Phys. Commun. 14 (1978) 13.
[2] J.C. Slater, in: Computational methods in band theory, eds. P.M. Marcus, J.F. Janak and A.R. Williams (Plenum Press, New York, 1970) p. 447.
[3] K.H. Johnson, Advan. Quantum Chem. 7 (1973) 143.
[4] J.C. Slater, Advan. Quantum Chem. 6 (1972) 1.
[5] J.C. Slater and K.H. Johnson, Phys. Rev. B5 (1972) 844.
[6] F. Herman and S. Skillman, Atomic structure calculations (Prentice Hall, Englewood Cliffs, NJ, 1963).
[7] F.S. Ham and B. Segall, Phys. Rev. 124 (1961) 1786.
[8] J.-P. Desclaux, Comput. Phys. Commun. 1 (1969) 216.
[9] M. Klobukowski, Comput. Phys. Commun. 25 (1982) 29.

Computer Physics Communications 25 (1982) 57–62
North-Holland Publishing Company

# VECTORIZING THE MONTE CARLO ALGORITHM FOR LATTICE GAUGE THEORY CALCULATIONS ON THE CDC CYBER 205

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*Control Data Limited, 179–199 Shaftesbury Avenue, London, WC2H 8AR, UK*

and

K.J.M. MORIARTY
*Department of Mathematics, Royal Holloway College, Egham, Surrey TW20 0EX, UK*

Received 6 August 1981

## PROGRAM SUMMARY

*Title of program*: LATTICE

*Catalogue number*: AARH

*Computer*: CDC CYBER 205; *Installation*: CYBERNET Data Center, Minneapolis, MN, USA (test run was executed on the system when it was being checked out)

*Operating system*: CYBER 200 O.S.

*Programming language used*: CYBER 200 FORTRAN

*High speed storage required*: 65–256 K (virtual memory system)

*Number of bits in a word*: 64

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 662

*Keywords*: lattice gauge theory, SU(4) gauge theory, SU($N$) gauge theory, Yang–Mills theory, non-Abelian gauge theory, non-perturbative effects, phase transitions, statistical mechanics, action per plaquette, Monte Carlo techniques, vector processors

*Nature of the physical problem*
The program calculates the average action per plaquette for SU(4) lattice gauge theory. Gauge theories on a lattice were originally proposed by Wilson [1] and Polyakov [2] for the regulation of the divergences of quantum field theory.

*Method of solution*
A Monte Carlo simulation of the system set up on a lattice (with varying numbers of sites per dimension considered) under an SU(4) gauge field, generates a series of field configurations. The method of Metropolis et al. [3] is used to achieve statistical equilibrium. Once in a state of statistical equilibrium any order parameter for the system can be measured. The vector capability of the CDC CYBER 205 is exploited to significantly reduce the time over that used on a scalar machine.

*Restrictions on the complexity of the program*
The storage required is dependent on the number $n$ of dimensions and the number $l$ of lattice sites along each dimension. The arrays in the program that usually have the largest dimensions are dimensioned to $nl^n$ (i.e. the number of links involved in the lattice). The execution time increases with the number of links and the number of Monte Carlo iterations. The code will only execute on CDC CYBER 200 computers due to usage of extensions of FORTRAN which amount to syntax for vector operations.

*References*

[1] K.G. Wilson, Phys. Rev. D10 (1974) 2455.
[2] A.M. Polyakov, unpublished.
[3] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.

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Computer Physics Communications 25 (1982) 63–71
North-Holland Publishing Company

# FERMI-SURFACE: A PACKAGE TO DISPLAY PERSPECTIVE DRAWINGS OF FERMI SURFACES IN CUBIC SYSTEMS *

Pratap C. PATTNAIK, Philip H. DICKINSON and John L. FRY
*Department of Physics, University of Texas, Arlington, TX 76019, USA*

Received 5 August 1981

## PROGRAM SUMMARY

*Title of program*: FERMI-SURFACE

*Catalogue number*: AARQ

*Computer*: DEC-20; *Installation*: Academic Computing Center, University of Texas at Arlington, Arlington, TX 76019, USA

*Operating system*: TOPS-20 Monitor 4

*Programming language used*: Fortran 20(5A) (this is a subset of Fortran-77)

*High speed storage used*: 60 474 words

*No. of bits in a word*: 36

*Overlay structure*: none required

*Other peripherals used*: graphic terminal and disc or card reader

*No. of cards in the combined program and test deck*: 2083

*Keywords*: Fermi surface, solid state physics, band structure, 3-D graphics

*Nature of the problem*
A perspective drawing of the Fermi surface in cubic systems.

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* Supported by The Robert A. Welch Foundation.

Computer Physics Communications 25 (1982) 73–80
North-Holland Publishing Company

# A VECTORIZABLE EIGENVALUE SOLVER FOR SPARSE MATRICES

L.C. BERNARD and F.J. HELTON
*General Atomic Company, San Diego, CA 92138, USA*

Received 4 December 1979; in revised form 28 August 1981

## PROGRAM SUMMARY

*Title of program*: EIGVEC

*Catalogue number*: AARI

*Computer*: CRAY-1; *Installation*: Magnetic Fusion Energy Computer Center, Livermore, USA

*Operating system*: LTSS

*Programming language used*: FORTRAN

*High speed store required*: 21822 + commons

*Number of bits in a word*: 64

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: 4 disk files

*Number of statements in combined program and test deck*: 1734

*Keywords*: general purpose, numerical mathematics, eigenvalue problem, inverse vector iteration, block matrix, symmetric matrix, sparse matrix, pattern recognition, vectorization

*Nature of the problem*
This package solves the generalized eigenvalue problem $Ax = \lambda Bx$, a problem which arises often, for example, in: physics, mechanics and chemistry. Here, $A$ and $B$ have a global block diagonal form and fine sparse structure as found in two-dimensional problems with a finite element approach.

*Method of solution*
Any mode can be obtained by first shifting the spectrum, then using inverse vector iteration to converge toward the lowest eigenvalue in absolute value. The Cholesky decomposition of $A$ is efficiently done using vectorization. Sparse matrix techniques reduce I/O requirements and improve the Cholesky decomposition in some cases.

*Restrictions of the complexity of the problem*
Both matrices, $A$ and $B$, must be real symmetric, and $B$ must be positive-definite. Both must have the same sparsity pattern.

*Unusual features of the program*
The program uses two subroutines written in assembly language for vectorization. The nonstandard FORTRAN statement, NAMELIST, is used.

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Computer Physics Communications 25 (1982) 81–85
North-Holland Publishing Company

# FORTRAN PROGRAM FOR THE INTEGRAL OF THREE SPHERICAL HARMONICS

Adelsindo LIBERATO de BRITO
*Federal University of Paraíba, Department of Physics, João Pessoa, Paraíba, Brasil*

Received 3 October 1980

## PROGRAM SUMMARY

*Title of program*: F3Y

*Catalogue number*: AAQQ

*Computer*: IBM-1130; *Installation*: Federal University of Paraíba, João Pessoa

*Operating system*: MONITOR

*Programming language used*: FORTRAN 4

*High speed storage required*: 1646 words

*No. of bits in a word*: 16

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 121

*Keywords*: molecular physics, spherical harmonics, Condon–Shortley parameters

*Nature of the physical problem*
First-principles calculations on atoms and molecules usually express the many-body wave function $\psi$ in terms one-particle states of the form $\phi(r) = R_{nl}(r)Y_{lm}(\theta, \phi)$, and the evaluation of physical quantities from $\psi$ invariably requires a considerable amount of manipulation of the $Y_{lm}(\theta, \phi)$.

Integrals of products of spherical harmonics appear in the evaluation of Coulomb matrix elements in atomic calculations [1,2], and they are closely related to the addition of angular momenta [3]. We therefore present a FORTRAN program for calculating these integrals.

*Method of solution*
There have been derived [4] two identities that provide substantial shortcuts to many of the more complicated results involving spherical harmonics.

The formula for the integral of three spherical harmonics is usually obtained by expressing the $Y_{lm}$ in terms of associated Legendre functions and integrating by parts as many times as necessary (Gaunt's formula [5]).

Our approach makes use of one of the quoted identities.

*Typical running time*
The maximum running time for one value of the integral with the absolute values of the arguments all smaller than 5 was 100 ms on the IBM-1120.

*References*

[1] E.U. Condon and G.H. Shortley, The theory of atomic spectra (Cambridge Univ. Press, Cambridge, England, 1953).
[2] J.C. Slater, Quantum theory of matter (McGraw-Hill, New York, 1968).
[3] A.R. Edmonds, Angular momentum in quantum mechanics (Princeton Univ. Press, Princeton, N.J., 1960) in particular eq. (4.6.4).
[4] A. Liberato de Brito, T.P. Eggarter, Intern. J. Quantum Chem. 17 (1980) 459.
[5] A. Gaunt, Phil. Trans. Roy. Soc. Sec. A228 (1929) 192.

Computer Physics Communications 25 (1982) 87–95
North-Holland Publishing Company

# COULOMB FUNCTIONS ANALYTIC IN THE ENERGY

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Received 1 July 1981

The Coulomb functions $f(\epsilon, l; \rho)$ and $g(\epsilon, l; \rho)$ are required for applications of quantum defect theory; $\epsilon$ is the $Z$-scaled energy, $l$ the angular momentum quantum number and $\rho$ the $Z$-scaled radial coordinate. The functions $f$ and $g$ are analytic in $\epsilon$. Power-series expansions are used to compute $f$ and $g$ and their derivatives with respect to $\rho$. The computed value of the Wronskian gives an indication of the accuracy achieved.

## PROGRAM SUMMARY

*Title of program*: COULAN

*Catalogue number*: AAJJ

*Computer*: IBM 360/195; Installation: Rutherford Laboratory

*Operating system*: HASP–MVT

*Programming language used*: FORTRAN

*High speed storage required*: 4 Kbytes

*Number of bits in a word*: 64

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: VDU terminal, line printer

*Number of cards in combined program and test deck*: 337

*Keywords*: Coulomb functions, quantum defect theory

*Nature of the physical problem*
Quantum defect theory enables one to express values for various properties of atomic systems in terms of quantities which vary slowly as functions of the energy [1]. In using the theory for ab-initio calculations, one requires the Coulomb functions $f(\epsilon, l; \rho)$ and $g(\epsilon, l; \rho)$ which are analytic in the energy variable $\epsilon$. A program is provided for the computation of these functions.

*Method of solution*
Power-series expansions are used.

*Restrictions on the complexity of the problem*
The computed value of the Wronskian gives an indication of the accuracy achieved. For the test run the fractional error in the Wronskian is not larger than 3.3E–09.

*Typical running time*
About 5 ms to calculate two linearly independent Coulomb functions, and their derivatives, for one energy, one angular momentum, one radial distance.

*References*
[1] M.J. Seaton, J. Phys. B11 (1978) 4067.

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Computer Physics Communications 25 (1982) 97–110
North-Holland Publishing Company

# A NON-ITERATIVE METHOD FOR SOLVING PDE's ARISING IN ELECTRON SCATTERING

E.C. SULLIVAN and A. TEMKIN
*NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA*

Received 10 July 1981

## PROGRAM SUMMARY

*Title of program*: SEPDE

*Catalogue number*: AANP

*Computer*: IBM 360/91; *Installation*: Goddard Space Flight Center, Greenbelt, MD 20771

*Operating system*: HASP/OS MVT

*Programming language used*: Fortran IV

*High speed storage required*: see note added in proof

*Number of bits in a word*: 32

*Overlay structure*: none

*Number of magnetic tapes required*: none

*Other peripherals used*: line printer, discs or magnetic tape

*No. of cards in combined program and text deck*: 356

*Keywords*: atomic, molecular, electron scattering, Schrödinger equation, electron–atom scattering, electron–molecule scattering, partial differential equations, non-iterative block solution, large linear systems, (coupled) elliptic partial differential equations, rectangular boundary conditions, non-iterative partial differential equation method

*Nature of the physical problem*
The major approach to (low energy)scattering of electrons from atomic and, more recently, molecular systems comes from decomposing the scattering wave function into partial waves. Rather than expand the solutions of the partial wave equations to obtain a coupled set of ordinary integro–differential equations, the SEPDE program solves the partial wave equations directly, avoiding the convergence problems encountered with arbitrarily truncating the expansion of each specific partial wave equation.

*Method of solution*
The partial differential equation is approximated by a linear system of equations. The system of equations is arranged in a block tridiagonal form and the solution of the system obtained directly rather than iteratively. Since the method of solution uses matrices dimensioned according to the block size, one avoids the requirement of banded methods that coefficients of the matrix within the band be in the computer memory at the same time.

*Restrictions on the complexity of the program*
The program is restricted to two-dimensional elliptic partial differential equations for rectangular regions. The program will handle multiple boundary conditions and systems of coupled equations. The computer memory requirements depend on the grid size chosen and the number of equations to be solved. The dimensioning for a given problem is done in one BLOCK DATA initializing routine. The user must also provide a subroutine which evaluates the coefficients of the block diagonal matrices; analogous to the way a derivative routine must be provided for routines which solve systems of ordinary differential equations.

*References*
[1] A. Temkin, in: Autoionization, ed. A. Temkin (Mono Book, Baltimore, 1966) p. 55.

2] A. Temkin, Phys. Rev. 126 (1962) 130.
3] A. Temkin and E. Sullivan, NASA Technical Note TN D-1702 (1963).
4] N. Chandra and A. Temkin, Phys. Rev. A13 (1976) 188.
[5] A. Temkin, in: Symp. on Electron–molecule collisions, Univ. of Tokyo (1979) p. 55.
[6] J.J. Dongarra et al., Linpack user's guide (SIAM, Philadelphia, 1979).

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Computer Physics Communications 25 (1982) 111
North-Holland Publishing Company

# ERRATUM NOTICE

*Title of paper*: PLATTSUM: a FORTRAN program that evaluates electrostatic lattice sums by the planewise summation method

*Authors*: J.A. Hernando and V. Massidda

*Reference*: Comput. Phys. Commun. 22 (1981) 13

*Title of program*: PLATTSUM

*Catalogue number*: ABVT

Computer Physics Communications 25 (1982) 125–139
North-Holland Publishing Company

# DFPOT – A PROGRAM FOR THE CALCULATION OF DOUBLE FOLDED POTENTIALS

J. COOK *

*Wheatstone Laboratory, King's College, Strand, London, WC2R 2LS, UK*

Received 31 July 1981

## PROGRAM SUMMARY

*Title of program*: DFPOT

*Catalogue number*: ABQP

*Computer*: IBM 360/195; *installation*: Rutherford laboratory

*Operating system*: HASP

*Programming language used*: FORTRAN IV

*High speed storage required*: 81768 bytes

*No. of bits in a word*: 64

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer, disc drive (optional), card punch (optional)

*No. of cards in combined program and test deck*: 964

*Keywords:* double folded potentials, transition potentials, convolution, Fourier transforms, elastic and inelastic scattering, density dependent interactions

*Nature of physical problem*
The program calculates double folded potentials for use in nuclear scattering problems by integrating a nucleon–nucleon interaction over the density distributions of the two colliding nuclei as described in ref. [1]. Potentials for elastic, inelastic and other scattering processes may be generated by appropriate choice of the interaction and the densities. In addition to a wide range of density independent interactions, a restricted class of density dependent interactions may also be employed.

*Method of solution*
The potential is calculated by making multipole expansions of the densities and performing the integration in momentum space by a Fourier transform technique.

*Restrictions on the complexity of the problem*
The program has been written to be very general with few restrictions. The main restriction is that only a limited type of density dependent interactions may be used. Other minor restrictions are described fully in the long write-up.

*Typical running time*
Using the IBM H-compiler the test calculation described in section 6 of the long write-up took 16.6 s to compile, 0.4 s to link-edit and 2.1 s to execute.

## Reference

[1] G.R. Satchler and W.G. Love, Phys. Rep. 55 (1979) 183.

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* Present address: Department of Physics, Florida State University, Tallahassee, FL 32306, USA.

Computer Physics Communications 25 (1982) 141–148
North-Holland Publishing Company

# PROFILE: A CODE FOR EVALUATING LINE PROFILE SHAPES FOR OPTICALLY THICK EXPANDING PLASMAS

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*Laser Physics Laboratory, Department of Engineering Physics, Research School of Physical Sciences, The Australian National University, Canberra, ACT 2600, Australia*

Received 1 August 1981

## PROGRAM SUMMARY

*Title of program*: PROFILE

*Catalogue number*: AARK

*Computer*: UNIVAC 1100/82; *Installation*: The Australian National University, Canberra

*Also operable on*: *Computer*: ICL 1904/S; *Installation*: University of Hull, England
*Computer*: CDC 7600; *Installation*: University of Manchester Regional Computer Centre, England

*Operating system*: EXEC 1100

*Programming language used*: FORTRAN

*High speed store required*: 12 800 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer, card reader

*No. of cards in combined program and test deck*: 1149

*Keywords*: radiative transfer, line profile, opacity, fine structure, plasma, spectroscopy, atomic, astrophysics

*Nature of physical problem*
The shape of a spectral line profile emitted from a plasma can be a sensitive indicator of the parameters of the plasma. Traditionally, optically thin profiles have been used for plasma measurements, but optically thick profiles are now increasingly being investigated as diagnostics for dense (e.g. laser-produced plasmas) or large (e.g. the solar corona) plasmas.

*Method of solution*
PROFILE calculates the shape of line profiles emitted from optically thick plasmas. Processes which are modelled include the effect of bulk plasma motion and fine structure broadening, as well as absorption. The equation of radiative transfer is solved at wavelength points across the profile for input plasma parameters such as the plasma velocity variation and the emissivity and absorption coefficient as a function of distance.

*Restrictions on the complexity of the problem*
The code is optimised for speed by assuming analytic formulae for the local broadening profiles. However, even complicated local broadening profiles can usually be approximated to a suitable form for the code.

*Typical running time*
For execution on the UNIVAC 1100/82, from 0.5 to 20 s depending on the input data.

*Unusual features of the programs*
PROFILE is written in standard FORTRAN IV.

Computer Physics Communications 25 (1982) 149–157
North-Holland Publishing Company

# PROGRAMS FOR THE COUPLING OF SPHERICAL HARMONICS

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*Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-8400 Regensburg, Fed. Rep. Germany*

Received 5 June 1981

## PROGRAM SUMMARY

*Title of program*: YLM-COUPLING

*Catalogue number*: AARL

*Computer*: TR440; *Installation*: Rechenzentrum der Universität Regensburg, Fed. Rep. Germany

*Operating system*: BS3 MV 19

*Programming language used*: FORTRAN IV

*High speed storage required*: approx. 12 000 words

*No. of bits in a word*: 48

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: card reader, line printer (for test)

*No. of cards in combined program and test deck*: 1141

*Keywords*: spherical harmonics, Gaunt coefficient, Condon–Shortley coefficient, coupling of two orbital angular momenta

*Nature of the physical problem*
The subroutines GAUNT and RECYLM allow the linearization of the product of two spherical harmonics according to the following formula

$$Y_{l_2}^{m_2 *}(\Omega)\, Y_{l_3}^{m_3}(\Omega) = \sum_{l_1} \langle l_3 m_3 | l_2 m_2 | l_1 m_3 - m_2 \rangle \, Y_{l_1}^{m_3 - m_2}(\Omega).$$

The summation limits of the $l_1$ summation are determined by certain selection rules for the Gaunt coefficients $\langle l_3 m_3 | l_2 m_2 | l_1 m_3 - m_2 \rangle$.

*Method of solution*
The subroutine GAUNT computes a whole string of Gaunt coefficients $\langle l_3 m_3 | l_2 m_2 | l_1 m_3 - m_2 \rangle$ for all allowed $l_1$ values ($l_2$, $m_2$, $l_3$ and $m_3$ are fixed input quantities) using their representation in terms of $3jm$-symbols. The $3jm$-symbols are computed using a homogeneous 3-term recurrence relation derived by Schulten and Gordon [1]. The computational algorithm used is apart from certain modifications the same as that developed by Schulten and Gordon [1].

The subroutine RECYLM computes a string of spherical harmonics $Y_l^m$ for all $l$ with $l^{\min} = |m| \leqslant l \leqslant l^{\max}$ ($m$ and $l^{\max}$ are input quantities) recursively using their homogeneous 3-term recurrence relation in $l$ [2]. Both programs use DOUBLE PRECISION arithmetic for floating point numbers.

*Typical running time*
Approximately 1 ms per Gaunt coefficient for the string $\langle 15\ 0 | 15\ 0 | l\ 0 \rangle$, approx. 3 ms for the string $\langle 15\ 15 | 15\ 15 | l\ 0 \rangle$ and approx. 4.5 ms for the string $\langle 8\ {-5} | 10\ 7 | l\ {-12} \rangle$.

Approximately 1.3 ms per spherical harmonic for the string $Y_l^0$, $0 \leqslant l \leqslant 15$, and approx. 1.5 ms for the string $Y_l^{-2}$, $2 \leqslant l \leqslant 5$.

To make these absolute numbers comparable: On the TR 440 one evaluation of DSQRT requires approx. 0.43 ms.

*Unusual features of the program*
In order to avoid complex arithmetic the azimuth angle $\phi$ is set equal to zero, i.e. RECYLM calculates a string of spherical harmonics $Y_l^m(\theta, 0)$.

In order to prevent overflow or underflow two DOUBLE PRECISION variables HUGE and TINY have to be defined.

*References*

[1] K. Schulten and R.G. Gordon, Comput. Phys. Commun. 11 (1976) 269.
[2] A. Messiah, Quantum mechanics (North-Holland, Amsterdam, 1961) p. 495.

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Computer Physics Communications 25 (1982) 159–176
North-Holland Publishing Company

# PROGRAMS FOR THE DYNAMIC SIMULATION OF LIQUIDS AND SOLIDS
## II. MDIONS : RIGID IONS USING THE EWALD SUM

N. ANASTASIOU and D. FINCHAM
*Department of Chemistry, Royal Holloway College, Egham, Surrey, TW20 0EX, UK*

Received 24 August 1981

## PROGRAM SUMMARY

*Title of program*: MDIONS

*Catalogue number*: AARM

*Computer*: Cray-1; *Installation*: S.E.R.C. Daresbury Laboratory

*Operating system*: COS 1.09

*Programming language used*: FORTRAN IV

*High speed storage required*: 57203 words

*No. of bits in a word*: 64

*No. of magnetic tapes required*: none

*Other peripherals used*: disc files may be used to store restart configurations

*No. of cards in combined program and test deck*: 1826

*Keywords*: ionic liquids, molten salts, molecular dynamics, liquid simulation, Ewald sum

*Nature of physical problem*
Study of the thermodynamic, structural and dynamic properties of ionic solids or liquids, or mixtures thereof.

*Method of solution*
A system of a few hundred ions in periodic boundary conditions is simulated. The equations of motion are solved in a series of time steps at each of which the force on each ion due to its interaction with the other ions in the system is found. The non-Coulomb interaction is parametrised in the Born–Mayer–Huggins form. The Coulomb interaction is handled by means of the Ewald sum. When the system is in thermal equilibrium thermodynamic measurements are made by averaging over time. The radial distribution functions and structure factors can be found, and also the mean square displacements of the ions.

*Restrictions on the complexity of the problem*
The program becomes inefficient when systems of more than about a thousand ions are to be simulated.

*Typical running time*
The complete test job of 1401 steps took 354 s on the Cray-1.

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# PROGRAMS FOR THE DYNAMIC SIMULATION OF LIQUIDS AND SOLIDS
## II. MDIONS : RIGID IONS USING THE EWALD SUM (VECTORISED VERSION ON THE CRAY-1)

D. FINCHAM
*Department of Chemistry, Royal Holloway College, Egham, Surrey TW20 0EX, UK*

Received 24 August 1981

## PROGRAM SUMMARY

*Title of program*: MDIONS (VECTORISED)

*Catalogue number*: AARN

*Computer*: Cray-1; *Installation*: S.E.R.C. Daresbury Laboratory

*Operating system*: COS 1.09

*Programming language used*: Cray Fortran

*High speed storage required*: 46550 words

*No. of bits in a word*: 64

*No. of magnetic tapes required*: none

*Other peripherals used*: disc files may be used to store restart configurations

*No. of cards in combined program and test deck*: 1530

*Reference to other published version of this program*:

*Catl. no.*: AARM; *title*: MDIONS; *ref. in CPC*: 25 (1982) 159.

*Keywords*: ionic liquids, molten salts, molecular dynamics, liquid simulation, Ewald sum

*Nature of physical problem*
Study of the thermodynamic, structural and dynamic properties of ionic solids or liquids, or mixtures thereof.

*Method of solution*
A system of a few hundred ions in periodic boundary conditions is simulated. The equations of motion are solved in a series of time steps at each of which the force on each ion due to its interaction with the other ions in the system is found. The non-Coulomb interaction is parametrised in the Born–Mayer–Huggins form. The Coulomb interaction is handled by means of the Ewald sum. When the system is in thermal equilibrium thermodynamic measurements are made by averaging over time. The radial distribution functions and structure factors can be found, and also the mean square displacements of the ions.

*Restrictions on the complexity of the problem*
The program becomes inefficient when systems of more than about a thousand ions are to be simulated.

*Typical running time*
To reproduce the complete test run of the original version takes 164 s.

*Unusual features of the program*
The program is an adaptation of the original, standard, version to take advantage of the vector-processing facilities of the Cray. Some features of the compiler, compatible with Fortran 77, are adopted to aid the user.

*Reference*

[1] N. Anastasiou and D. Fincham, Comput. Phys. Comm. 25 (1982) 159.

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Computer Physics Communications 25 (1982) 181–191
North-Holland Publishing Company

# MAGNETIC FIELD, VECTOR POTENTIAL AND THEIR DERIVATIVES DUE TO CURRENTS IN CLOSED POLYGONS OF WIRE

D.K. LEE

*Computer Sciences Division at Oak Ridge National Laboratory *, Oak Ridge, TN 37830, USA*

Received 1 May 1981

## PROGRAM SUMMARY

*Title of program*: BWIRE

*Catalogue number*: AARP

*Computer*: CDC-7600; *Installation*: National Magnetic Fusion Energy Computer Center, Lawrence Livermore National Laboratory, University of California, Livermore, CA 94550

*Operating system*: Livermore Time Sharing System (LTSS)

*Programming language used*: FORTRAN IV

*High speed storage required*: 10775 words

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: none

*No. of cards in program and test deck*: 633

*Keywords*: magnetic field, magnetic vector potential, partial derivatives, orthogonal transformation, scale factor, transition matrix

*Nature of problem*
The program evaluates the magnetic field, the magnetic vector potential and their partial derivatives for two types of magnetic sources: (1) current-carrying straight wire of finite length and (2) current-carrying closed polygon (not necessarily plane) consisting of three or more straight wires of finite length.

*Method of solution*
Explicit expressions for the magnetic field, the magnetic vector potential, their partial derivatives and many other related quantities are derived analytically in the Cartesian coordinate system for a current-carrying straight wire of finite length. Orthogonal transformation is employed to obtain the results in other orthogonal coordinates.

*Restrictions*
The observation point (where the magnetic field and other quantities are to be evaluated) is singular if it is collinear with the straight wire, and hence such a point should be avoided. The present program gives the results in four different orthogonal coordinate systems: Cartesian, cylindrical, spherical and local toroidal. For other orthogonal systems, one needs only a minor modification which involves evaluation of scale factors and transition matrix elements. More general coordinates require more extensive modification of the formulation.

*Typical running times*
The program for the test case includes seven subroutines, but only one or two will be necessary in almost all applications. This test case used 13.85 s to compile, load and execute. For a current loop consisting of four straight wires, a single execution time for calculation of the magnetic quantities ranges from $0.55 \times 10^{-4}$ s to $2.66 \times 10^{-4}$ s, depending on which subroutine is used.

*Unusual features of the program*
The program is fairly fast and accurate, since all quantities are derived analytically and precisely in simple closed forms and exact identities are utilized to the greatest possible extent to make the numerical procedure as efficient as possible.

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* Operated by Union Carbide Corporation under contract W-7405-eng-26 with the US Department of Energy.

Computer Physics Communications 25 (1982) 193–205
North-Holland Publishing Company

# CALCULATION OF X-RAY ABSORPTION NEAR-EDGE STRUCTURE, XANES

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and

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*Topexpress Ltd., Cambridge CB5 8AF, UK*

Received 27 October 1981

## PROGRAM SUMMARY

*Title of program*: DLXANES

*Catalogue number*: AARR

*Computer*: NAS 7000; *Installation*: Daresbury Laboratory

*Operating system*: HASP

*Programming language*: FORTRAN IV (IBM)

*High speed storage required*: 304 Kbytes

*No. of bits per word*: 32

*Overlay structure*: none

*Other peripherals used*: none

*No. of magnetic tapes required*: none

*No. of cards in program and test deck*: 2740

*Keywords*: X-ray absorption, near-edge, K-shell, core level, excited electron, multiple scattering, solids, ordered, disordered, surfaces, local structure

*Nature of problem*
To calculate the transition rate for X-ray absorption close to threshold for condensed systems in which the local atomic arrangement may be complex (e.g. crystals with many atoms per unit cell, disordered systems, surfaces, etc.). We are concerned with the so-called X-ray absorption near-edge structure (XANES), within approximately 50 eV of the edge.

C-782

*Method of solution*

The transition rate is calculated within the dipole approximation. An atomic contribution is identified, together with modifications arising from multiple scattering of the excited electron by the surrounding atoms. This multiple scattering is calculated by means of a real space cluster approach, which is considerably more flexible than band structure methods. Structural symmetry (rotation/reflection) is exploited if it exists, but is not required.

*Restrictions*

The program is currently restricted to spectra involving core levels of s-symmetry, i.e. K, $L_1$ edges, etc. (More generally, the restriction is to spectra in which there is no interference between the $l+1$ and $l-1$ channels coupled by the dipole selection rule to a core level of angular momentum $l$.)

Computer Physics Communications 25 (1982) 207
North-Holland Publishing Company

## ERRATUM NOTICE

*Title of paper*: Bessel functions $I_\nu(z)$ and $K_\nu(z)$ of real order and complex argument

*Author*: J.B. Campbell

*Reference*: Comput. Phys. Commun. 24 (1981) 97

*Title of program*: BESSIK

*Catalogue number*: AAQZ

C-784

Computer Physics Communications 25 (1982) 223–236
North-Holland Publishing Company

# A PROGRAM FOR ANALYSING THE RYDBERG SERIES OF HIGHLY EXCITED DISCRETE SPECTRA BY M.Q.D.T.

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*Laboratoire Aimé Cotton, CNRS II, Campus d'Orsay, Bâtiment 505, 91405 Orsay Cedex, France*

Received 8 September 1981

## PROGRAM SUMMARY

*Title of program*: MQDTAC

*Catalogue number*: AANQ

*Computer*: UNIVAC 1110; *Installation*: Paris-Sud Informatique, Université Paris XI, 91405 Orsay Cedex

*Operating system*: EXEC VIII

*Programming language used*: Fortran 77

*High speed storage required*: 24557 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: printer, card reader

*No. of cards in combined program and test deck*: 2362

*Keywords*: atomic physics, Rydberg levels, multichannel quantum defect theory

*Nature of physical problem*

A collision theory analysis of highly perturbed spectra has been recently developed by Fano [1] which relies on Seaton's Multichannel Quantum Defect Theory (M.Q.D.T.) [2]. Various photoabsorption data relevant to discrete, autoionization and continuous spectra can be expressed in terms of three sets of meaningful parameters.

The program enables several atomic quantities to be computed in terms of these M.Q.D.T. parameters ($\mu_\alpha$, $U_{i\alpha}$, $D_\alpha$). The $\mu_\alpha$ and $U_{i\alpha}$ parameters relevant to the calculation of energies are determined from data on perturbed Rydberg series while the $D_\alpha$ needed to calculate oscillator strengths are given as input. Graphical analysis of perturbed Rydberg series is performed by means of Lu–Fano curves [3].

*Method of solution*

The $\mu_\alpha$ and $U_{i\alpha}$ parameters are optimized through an iterative process according to one of the following quality criteria (available as input):

a) minimisation of the rms deviation between theoretical and experimental energies of discrete levels,

b) minimisation of a sum of determinants characteristic of the M.Q.D.T.

*Restrictions on the complexity of the problem*

The maximum number of series converging to the first ionisation limit is limited to 3.

– Autoionisation profiles are computed for the levels lying in the energy range between the first two limits of ionisation,

– Branching ratio is given for the case of only two different ionic states (noble gases).

*References*

[1] U. Fano, J. Opt. Soc. Am. 65 (1975) 979.
[2] M.J. Seaton, Proc. Phys. Soc. (London) 88 (1966) 801.
[3] K.T. Lu and U. Fano, Phys. Rev. A2 (1970) 81.

Computer Physics Communications 25 (1982) 237–252
North-Holland Publishing Company

# NUCORE – A SYSTEM FOR NUCLEAR STRUCTURE CALCULATIONS WITH CLUSTER–CORE MODELS

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and

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Received 5 October 1981

## PROGRAM SUMMARY

*Title of program*: NUCORE

*Catalogue number*: AARQ

*Computer*: IBM 4341; *Installation*: Information and Computing Service, SHELL C.A.P.S.A., Buenos Aires

*Operating system*: DOS/VSE (R2.0 PUT 8005)

*Programming language used*: FORTRAN IV (5746-LM3-F03)

*High-speed storage required*: 128000 words

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: one

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 3546

*CPC library subprograms used*:

*Catalogue number*: ACWH;

*Title*: MINUIT; *Ref. in CPC*: 10 (1975) 343

*Keywords*: cluster phonon model, minimization, nuclear energy levels, reduced quadrupole electric transition probabilities, reduced

dipole magnetic transition probabilities, electric quadrupole moments, magnetic dipole moments, mixing ratios, branching ratios, total lifetimes

*Nature of Physical problem*
Calculation of nuclear energy levels and their electromagnetic properties, modelling the nucleus as a cluster of a few particles and/or holes interacting with a core which in turn is modelled as a quadrupole vibrator (cluster–phonon model) [1]. The members of the cluster interact via quadrupole–quadrupole and pairing forces.

*Method of solution*
The Hamiltonian matrix is diagonalized taking single-particle energies and interaction strength constants as adjustable parameters determined by fitting calculated to experimental energy levels through chi-square minimization. The resulting eigenvalues and eigenvectors are used to calculate electromagnetic properties of the levels.

*Restrictions on the complexity of the program*
1) The subroutine PHONON and CO2H1P are restricted to a maximum number of two phonons. The dimensions of the arrays depend rather strongly on this. It must be pointed out that for a given number of phonons the dimensions are also modified according to the different number of single-particle orbitals needed for different nuclei.
2) The first run of program no. 2 depends essentially on the use of the system MINUIT [2]. Modification of the code might be needed with alternative minimizing routines.
3) The actual code is designed for diagonalizing routines using only non-zero matrix elements.
4) The present version of the code applies to cases in which only one level parity is implied. However, slight modifications allow the program to be used when both parities are involved.

*Typical running time*
The execution time is strongly problem dependent. The test runs, which involve the building and diagonalization of a 63 × 63 matrix with a total of 617 non-zero elements, and the computation of the electromagnetic properties for three calculated energy levels, require a total of 24 min (including 17 min of compilation time).

*Unusual features of the program*
To maximize the utility of the program, the following features are provided.
1) The MAIN is simple and most flexible with the "physics" included in routines. Thus, it can be adapted to manage different nuclear models within the same computational framework.
2) The routines are designed in such a way that they have non-dimensioned variables or variable-dimensioned ones, thus greatly reducing storage requirements.
3) The program permits the use of alternative routines to calculate radial integrals, to diagonalize matrices, and to minimize the desired functions.
4) The subroutine FCN is so implemented that it may be used without any minimization. Therefore, the same MAIN program is used to perform different tasks.

*References*
[1] C.A. Heras and S.M. Abecasis, Phys. Rev. C12 (1975) 1659.
[2] F. James and M. Roos, Comput. Phys. Commun. 10 (1975) 343.

Computer Physics Communications 25 (1982) 253–268
North-Holland Publishing Company

# HEVOL: A MONTE CARLO PROGRAM TO CALCULATE THE EVOLUTION OF STRUCTURE FUNCTIONS WITH THE INCLUSION OF HEAVY QUARK EFFECTS

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Received 15 July 1981

## PROGRAM SUMMARY

*Title of program*: HEVOL

*Catalogue number*: AAVH

*Computer*: CDC 7600; *Installation*: CINECA, Bologna
The program has also been run on the CDC 7600 at CERN, Geneva

*Operating system*: scope 2.1.5 and NOS/BE

*Programming language used*: FORTRAN IV EXTENDED

*High speed storage required*: 21 672 words – can be varied according to the choice of parameters

*No. of bits in a word*: 60

*Overlay structure*: none

*No. of magnetic tapes required*: none

*Other peripherals used*: line printer, permanent files on disk (the latter optionally, to save execution time)

*No. of cards in combined program and test deck*: 1973

*Keywords*: Monte Carlo generation, quantum chromodynamics, structure function evolution, leading logarithm approximation, heavy quark effects

*Nature of physical problem*
Calculation of the QCD evolution of structure functions including the effects of heavy quark production, with the immediate aim of determining relevant QCD parameters by least-square fits to experimental data

*Method of solution*
Monte Carlo generation of the QCD emission of quanta by a procedure developed in ref. [1].

*Typical running time*
In the test program set-up (singlet analysis of muon deep inelastic scattering data, 94 data points with $Q^2$ ranging from 2.8 to 200 GeV$^2$, minimum Bjorken's $x$ 0.04, $\Lambda \leqslant 0.5$ GeV, and charmed sea contribution calculated separately) 137 s of CDC 7600 time to process $4 \times 50\,000$ cascades for the calculation of kernels (which can be saved on disk for after use with the same data, or subset of them), and 0.03 s per call of the minimization program MINUIT (for convolutions done with 100$x$-bins). If non-singlet quantities only are needed the kernel calculation time reduces to about 15 s and the time per MINUIT call to 0.02 s, under the same conditions and minimum $x$ 0.25.

*Unusual features of the program*
Use of the CERN program library, and specifically of the minimization program MINUITS.

*References*

[1] R. Odorico, Phys. Lett. 102B (1981) 341.

C-788

Computer Physics Communications 25 (1982) 269–273
North-Holland Publishing Company

# LATTICE DYNAMICS OF ZINCBLENDE STRUCTURE COMPOUNDS USING A DEFORMABLE ION MODEL

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Received 1 October 1981

## PROGRAM SUMMARY

*Catalogue number*: ACUG

*Title of program*: Lattice dynamics of zincblende

*Computer*: CDC Cyber 173; *Installation*: University of Aarhus

*Operating system*: NOS ver.1.4-509/508-A

*Programming language*: FORTRAN IV

*High speed storage required*: 18 kwords

*No. of bits in a word*: 60

*Peripherals used*: lineprinter

*No. of cards*: 266

*CPC Library program used*:

*Catalogue number*: ACMP

*Title*: Lattice Dynamics of Zinc blende

*Ref. in CPC*: 16 (1979) 181

*Keywords*: solid state, semiconductor, lattice dynamics, phonons, dispersion curves, dynamical matrix, zincblende structure, diamond structure, deformable ion model

*Nature of physical problem*
Phonon frequencies and eigenvectors are calculated for a given wavevector $\boldsymbol{k}$.

*Method of solution*
The dynamical matrix is calculated within the deformable-ion-model approximation.

*Restrictions on the complexity of the program*
Zincblende and diamond structures only.

*Typical running time*
0.6 s per $\boldsymbol{k}$-vector.

omputer Physics Communications 25 (1982) 275–287
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# A FAST ALGORITHM FOR MONTE CARLO SIMULATIONS OF 4-d LATTICE GAUGE THEORIES WITH FINITE GROUPS

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*CERN, Geneva, Switzerland*

and

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Received 16 October 1981

## PROGRAM SUMMARY

*itle of program*: LATGAUGEMC

*atalogue number*: AAVI

*omputer*: CDC 7600; *Installation*: Brookhaven National aboratory, Upton, NY, 11973 and CERN, Geneva, Switzer-nd

he program is operable on any computer which has a word ructured memory with a wordlength of at least 28 bits, the ossibility to implement mask operations (bit by bit logical roduct) and circular left-shift, and FORTRAN IV

*perating system*: CDC Scope

*rogramming language used*: FORTRAN IV

*igh speed storage required*: 19634 D ($46262_8$) for the example

*o. of bits in a word*: 60

*verlay structure*: none

*eripherals used*: mass storage (amount depends on the appli-tion, 15741 D computer words in the example)

*No. of cards in combined program and test deck*: 393

*Keywords*: lattice gauge theory, discrete group, 4-dimensions, variable lattice size, periodic boundary conditions, Monte Carlo, Metropolis method

*Nature of the physical problem*

The program LATGAUGEMC generates configurations of the link-gauge variables of a 4-dimensional hypercubic lattice of linear extent 2, 4 or 8 with periodic boundary conditions. The link variables take values from any group where the number of group elements plus the number of elements equal to their own inverse is less than 128. The Monte Carlo method used to update the link variables is the Metropolis method [1]. The configurations generated by the program are representative of the ensemble of configurations on a finite lattice that defines the partition function of a lattice gauge field theory. They may be used to evaluate expectation values of functions of the gauge variables. The program has been used by the authors [2] to study the 4-dimensional SU(2) lattice gauge theory. It could be used for Monte Carlo simulations of other problems in statistical mechanics and particle physics.

C-790

*Unusual features of the program*

a) The group elements are labelled so that the operation of finding the inverse of any element is a single FORTRAN command.

b) The periodic boundary conditions on the lattice are implemented using shift and mask operations to perform the necessary modulo arithmetic.

These features result in a considerable increase in the speed of the Monte Carlo over other conventional methods.

*References*

[1] N. Metropolis, A.W. Rosenbluth, A.H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.

[2] C. Rebbi, Phys. Rev. D 21 (1980) 3350.
D. Petcher and D.H. Weingarten, Phys. Rev. D 22 (1980) 2465.
G. Bhanot and C. Rebbi, Nucl. Phys. B180 (1981) 469.
C.B. Lang, C. Rebbi, P. Salomonson and B.S. Skagerstam, Phys. Lett. 101B (1981) 173.

Computer Physics Communications 25 (1982) 289–295
North-Holland Publishing Company

# AUTOMATIC COMPUTATION OF BESSEL FUNCTION INTEGRALS

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Received 18 November 1981

## PROGRAM SUMMARY

*Title of program*: HANKEL

*Catalogue number*: AART

*Computer*: IBM 3033; *Installation*: University of Leuven, Computing Centre.

*Operating system*: OS/360

*Programming language used*: FORTRAN IV

*High speed storage required*: 8910 words

*No. of bits in a word*: 32

*Overlay structure*: none

*Peripherals used*: line printer (only for the test run)

*No. of cards in combined program and test deck*: 1413

*Keywords*: Bessel function, integral over an infinite interval, Hankel transform, Fourier transform, automatic numerical integration

*Nature of the physical problem*
Integrals over an infinite interval, involving Bessel functions, occur in many physical applications, especially as Hankel transforms in the solution of certain mixed boundary value problems [1]. In many cases these integrals cannot be computed analytically and must be evaluated numerically.

*Method of solution*
Using new approximations for the Bessel functions of the first kind $J_\nu(x)$, $0 \leqslant \nu \leqslant 10$ [2], integrals involving Bessel functions can be written as the sum of an integral over a finite interval and of a Fourier-sine and Fourier-cosine transform. For the computation of these three integrals, a lot of methods are available in the literature.

*Restrictions on the complexity of the problem*
Just as for other numerical integration routines, it is impossible to delineate the class of functions for which this algorithm is accurate, efficient and reliable. However, extensive testing has shown that it works very well for most Bessel function integrals arising in practical problem, if the Bessel function is the only oscillating factor of the integrand.

*Typical running time*
The computation of the 99 integrals in the test run took 7.48 s on the IBM 3033 (including the time required for the computation of the exact values of these integrals).

*References*

[1] I.N. Sneddon, Mixed boundary value problems in potential theory (North-Holland, Amsterdam; Interscience, New York, 1966).
[2] R. Piessens and M. Branders, Comput. Math. Appl. to be published.

C-792

Computer Physics Communications 25 (1982) 297–309
North-Holland Publishing Company

# ALPHA-DECAY HALF-LIFE SEMIEMPIRICAL RELATIONSHIPS WITH SELF-IMPROVING PARAMETERS

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Received 5 November 1981

## PROGRAM SUMMARY

*Title of program*: SEMIEMPIRICAL ALPHA HALF-LIFE

*Catalogue number*: ABQQ

*Computer*: IBM 370/135; *Installation*: Central Institute of Physics

*Operating system*: DOS/VS-310

*Programming language used*: FORTRAN IV

*High speed storage required*: 95 kbyte

*Number of bits per byte*: 8

*Overlay structure*: none

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 1511

*Keywords*: nuclear physics, radioactivity, alpha decay, semiempirical formulae, half-life

*Nature of the Physical Problem*
From the alpha decay $Q$-values, the partial half-life $T$ is estimated by using five semiempirical relationships [1–5]. The parameters of these formulae have been obtained from a fit with a given set of experimental data on four groups of alpha emitters: even–even, even–odd, odd–even and odd–odd.
For each nuclide only the strongest transition is considered and the data are automatically sorted into the four groups mentioned above. There are three options: one can use either the present set of parameter values, a new one given as input data, or new values computed by using a better set of experimental data (more accurate or more complete). For each group of nuclides, up to 8 (or 9) families of curves could be plotted, optionally, with the line printer. The calculated life-time can be compared either with the experimental one, if it is available, or with the time of ref. [5].

*Method of solution*
Only the additive parameters of the log $T$ formulae of refs. [1–4] are modified, by requesting a vanishing mean value of the absolute errors. The $B$-parameters defined in the ref. [5] are obtained by a parabolic least square fit.

*Restriction on the complexity of the problem*
The maximum number of alpha emitters in each of the four groups can not be larger than 300 in a given run. Up to 40 curves are accepted by the plotting subroutine.

*Typical running time*
For 100 alpha emitters, the tupical CPU running time on an IBM 370/135 ranges from 7 s (no plot) to 20 s (9 diagrams plotted) in the self-improving mode of operation and from 6 s to 18 s with the present set of parameters.

*Unusual features of the program*
The subroutines MZDPLT and MZDPFT could be used in other programs to plot a family of curves, or to make a bidimensional parabolic least squares fit, respectively.

*References*

[1] R. Taagepera and M. Nurmia, Ann. Acad. Sci. Fenn. Ser. A 78 (1961).
[2] V.E. Viola Jr. and G.T. Seaborg, J. Inorg. Nucl. Chem. 28 (1966) 741.
[3] K.A. Keller and H. Münzel, Z. Phys. 255 (1972) 419.
[4] P. Hornshøj, P.G. Hansen, B. Jonson, L. Ravn, L. Westgaard and O.N. Nielsen, Nucl. Phys. A230 (1974) 365.
[5] D.N. Poenaru, M. Ivaşcu and D. Mazilu, J. de Phys. Lett. 41 (1980) L-589.

omputer Physics Communications 25 (1982) 311–324
orth-Holland Publishing Company

# DELPHINE: PROGRAM TO BUNCH A DC BEAM THROUGH A TANDEM ACCELERATOR FOR INJECTION INTO A CYCLOTRON WITH SUPERCONDUCTING MAGNET *

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Received 25 October 1981; in revised form 21 December 1981

## PROGRAM SUMMARY

*itle of program*: DELPHINE

*atalogue number*: AARW

*omputer*: UNIVAC 1100; *Installation*: Centre de Calcul, entre de Recherches Nucléaires, 67037 Strasbourg, France

*rogramming language used*: FORTRAN V

*igh speed storage required*: 64000 words

*o. of bits in a word*: 36

*verlay structure*: none

*eripherals used*: card reader, line printer

*o. of cards in combined program and test deck*: 711

*eywords*: Gaussian and uniform distribution of phi, gaussian istribution of delta, bunching and rf frequency, energy moduation of the regrouper, equivalent drift length, bunching maix, harmonics and regrouping efficiency

*Nature of the physical problem*

Calculations of the ideal tensions and frequencies of the bunching elements in the transfer line to obtain a convenient emittance ellipse.

*Method of solution*

The solution is given by the subprogram NEXTPD, which gives the elements of the final vector by the following relation:

$$\begin{bmatrix} \phi_\mathrm{f} \\ \delta_\mathrm{i} \end{bmatrix} = \begin{bmatrix} 1 & \mathrm{BB} \\ -\mathrm{CC} * \mathrm{SP} & \mathrm{DD} \end{bmatrix} \begin{bmatrix} \phi_\mathrm{i} \\ \delta_\mathrm{i} \end{bmatrix},$$

$\begin{bmatrix} \phi_i \\ \delta_i \end{bmatrix}$ characterises the beam before entering the bunching system, and the first matrix on the right hand side of the equation is the general matrix describing the bunching parameters, whose significance is explained in the description of the program structure.

*Typical running time*

For execution 19 s in the UNIVAC 1100 time/sharing EXEC-multi-processor system.

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This work was performed under the auspices of GEPAS (Groupe d'Etudes pour l'Accélérateur de Strasbourg), Centre de Recherches Nucléaires, Strasbourg.

Computer Physics Communications 25 (1982) 347–387
North-Holland Publishing Company

# A GENERAL PROGRAM TO CALCULATE ATOMIC CONTINUUM PROCESSES INCORPORATING MODEL POTENTIALS AND THE BREIT-PAULI HAMILTONIAN WITHIN THE *R*-MATRIX METHOD

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Received 19 October 1981

## PROGRAM SUMMARY

*Title of program*: RMATRX STG1R

*Catalogue number*: AANR

*Computer*: CRAY-1; *Installation*: SRC, Daresbury Laboratory, Warrington

*Operating system*: COS 1.09

*Programming language used*: ANSI FORTRAN 66

*High speed storage required*: 169900 words

*No. of bits in a word*: 64

*Overlay structure*: none

*No. of magnetic tapes required*: 1 or 2

*Other peripherals used*: card reader, lineprinter, scratch disc store, permanent disc store

*No. of cards in source program*: 6047

*Card punching code*: EBCDIC

*Reference to other published version of this program:*

*Catalogue number*: AAHF

*Title*: A new version of RMATRX STG1

*Ref. in CPC*: 14 (1978) 367

*CPC Library subprograms used*:

*Catalogue numbers*: AANS, AANT, AANU, AANV

*Titles*: RMATRX STG2R, RMATRX RECUP, RMATRX RECUD, RMATRX STG3R

*Ref. in CPC*: this paper

*Keywords*: atomic, electron–atom, scattering, electron–ion, photoionization, polarizability, *R*-matrix, continuum, bound, de Vogelaere's method, radial integrals, RK integrals, model-potential, mass-correction, Darwin term, spin–orbit, pair-coupling, Breit–Pauli Hamiltonian, relativistic effects, fine structure levels

*Nature of the physical problem*
This program calculates all one-electron, two-electron and multipole radial integrals involving bound and continuum orbitals. These radial integrals enable the calculation of electron scattering and photoionization cross-sections for a general atomic system. Cross-sections between fine structure levels may be obtained by introducing relativistic effects through the Breit–Pauli Hamiltonian and pair-coupling [1]. The closed shell core of the target atom may be approximated by a model potential The bound orbitals are specified analytically. The continuum orbitals are calculated by the program. The integrals are stored on a magnetic tape or disc file for use by RMATRX STG3R [2].

*Method of solution*
The continuum orbitals are determined by integrating numerically a differential equation with a given potential using de Vogelaere's method and subject to *R*-matrix boundary conditions. The radial integrals are evaluated numerically using Simpson's rule.

*Restrictions on the complexity of the program*
The Schmidt orthogonalisation procedure may not be used i relativistic operators are included in the Hamiltonian. Consul

ubroutine SETDIM of RMATRX STG1R [2] for details of urrent dimensions.

*ypical running time*

The running time depends approximately on the square of ne number of bound orbitals, on the square of the number of ontinuum orbitals for each angular momentum and on the umber of continuum angular momenta. The test run took 15 s n the CRAY-1

*eferences*

] N.S. Scott and P.G. Burke, J. Phys. B 13 (1980) 4299.
] N.S. Scott and K.T. Taylor, this paper.

## PROGRAM SUMMARY

*itle of program*: RMATRX STG2R

*atalogue number*: AANS

*omputer*: CRAY-1; *Installation*: SRC, Daresbury Laboratory, arrington

*perating system*: COS 1.09

*rogramming language used*: ANSI FORTRAN 66

*igh speed storage required*: 183 881 words

*o. of bits in a word*: 64

*verlay structure*: none

*o. of magnetic tapes required*: 3

*ther peripherals used*: card reader, lineprinter, scratch disc ore, permanent disc store

*o. of cards in source program*: 10 141

*eference to other published version of this program*:

*atalogue number*: AAHG

*itle*: A new version of RMATRX STG2

*ef. in CPC*: 14 (1978) 367

*PC Library subprograms used*:

*atalogue numbers*: AANR, AANT, AANU, AANV

*itles*: RMATRX STG1R, RMATRX RECUP, RMATRX ECUD, RMATRX STG3R

*ef. in CPC*: this paper

*eywords*: atomic, electron–atom, scattering, electron–ion, otoionization, *R*-matrix, Hamiltonian matrix, ionic, Racah efficients, coefficient of fractional parantage, recoupling, anılar integral, continuum, bound, *LS*-coupling, long-range otentials, dipole matrix, model-potential, relativistic effects

*ature of the physical problem*

ne program reads the radial integrals stored on a magnetic tape or disc file by RMATRX STG1R [1]. It then calculates the Hamiltonian matrix, the asymptotic potential coefficients and dipole length and velocity matrices. These quantities are stored on magnetic tapes or disc files for use by RMATRX STG3R or RMATRX RECUP and RMATRX RECUD [1].

*Method of solution*

The calculation is carried out in *LS*-coupling. The angular integrals are carried out using the techniques of Racah algebra. These are then combined with the radial integrals evaluated in RMATRX STG1R [1]. If relativistic effects are to be included one proceeds to RMATRX STG3R via RMATRX RECUP and RMATRX RECUD.

*Restrictions on the complexity of the program*

See subroutine SETDIM of RMATRX STG2R [1] for details of current dimensions.

*Typical running time*

The running time depends on the square of the number of shells and the number of configurations included. The test run took 7 s on the CRAY-1.

*References*

[1] N.S. Scott and K.T. Taylor, this paper.

## PROGRAM SUMMARY

*Title of program*: RMATRX RECUP

*Catalogue number*: AANT

*Computer*: CRAY-1; *Installation*: SRC, Daresbury Laboratory, Warrington

*Operating system*: COS 1.09

*Programming language used*: ANSI FORTRAN 66

*High speed storage required*: 242 785 words

*No. of bits in a word*: 64

*Overlay structure*: none

*No. of magnetic tapes required*: 3

*Other peripherals used*: card reader, lineprinter, scratch disc store, permanent disc store

*No. of cards in source program*: 6148

*CPC Library subprograms used*:

*Catalogue numbers*: AANR, AANS, AANU, AANV

*Titles*: RMATRX STG1R, RMATRX STG2R, RMATRX RECUD, RMATRX STG3R

*Ref. in CPC*: this paper

*Keywords*: atomic, electron–atom, scattering, electron–ion, photoionization, *R*-matrix, spin–orbit, pair-coupling, inter-

mediate coupling, unitary transformation, term coupling coefficients, coefficients of fractional parantage, Racah coefficient.

*Nature of the physical problem*
This program reads Hamiltonian matrices and long-range potential coefficients calculated in *LS*-coupling by RMATRX STG1R [1]. Using this information it constructs matrix elements of the Breit–Pauli Hamiltonian and long-range potential coefficients in pair-coupling. These quantities are stored on magnetic tape or disc files for use by RMATRX RECUD and RMATRX STG3R [1].

*Method of solution*
Hamiltonian matrices and long range potential coefficients calculated in *LS*-coupling by RMATRX STG2R are transformed, by means of a unitary transformation to pair-coupling. Angular integrals of the spin–orbit operator are evaluated in *LSJ*-coupling using Racah algebra. These are added to the spin–orbit radial integrals originally calculated in RMATRX STG2R. These matrices are then transformed by means of a unitary transformation, to pair-coupling and added to the transformed matrices from RMATRX STG2R to form matrix elements of the Breit–Pauli Hamiltonian.

*Restrictions on the complexity of the program*
See subroutine SETDIM in RMATRX RECUP for details of current dimensions.

*Typical running time*
The running time depends on the number of channels, target states and configurations included. The test run took 3 s on the CRAY-1.

*Reference*
[1] N.S. Scott and K.T. Taylor, this paper.

## PROGRAM SUMMARY

*Title of program*: RMATRX RECUD

*Catalogue number*: AANU

*Computer*: CRAY-1; *Installation*: SRC, Daresbury Laboratory, Warrington

*Operating system*: COS 1.09

*Programming language used*: ANSI FORTRAN 66

*High speed storage required*: 238 527 words

*No. of bits in a word*: 64

*Overlay structure*: none

*No. of magnetic tapes required*: 3

*Other peripherals used*: card reader, lineprinter, scratch disc store, permanent disc store

*No. of cards in source program*: 1275

*CPC Library subprograms used*:

*Catalogue numbers*: AANR, AANS, AANT, AANV

*Titles*: RMATRX STG1R, RMATRX STG2R, RMATRX RECUP, RMATRX STG3R

*Ref. in CPC*: this paper

*Keywords*: atomic, electron–atom, scattering, electron–atom, photoionization, reduced dipole matrix, length, velocity, relativistic effects, intermediate coupling, pair-coupling, *R*-matrix

*Nature of the physical problem*
This program reads from magnetic tape or disc file, reduced dipole length and velocity matrices calculated in *LS*-coupling by RMATRX STG2R [1] and recoupling information calculated by RMATRX RECUP [1]. Using this information reduced dipole length and velocity matrices are evaluated in pair-coupling. These quantities are stored on magnetic tape or disc files to be used by RMATRX STG3R [1].

*Method of solution*
Reduced dipole length and velocity matrices calculated in *LS*-coupling are transformed to pair-coupling by means of a unitary transformation.

*Restrictions on the complexity of the program*
Consult subroutine SETDIM of RMATRX RECUD to determine current dimensions.

*Typical running time*
The running time depends on the number of channels and configurations. The test run took 7 s on the CRAY-1.

*Reference*
[1] N.S. Scott and K.T. Taylor, this paper.

## PROGRAM SUMMARY

*Title of program*: RMATRX STG3R

*Catalogue number*: AANV

*Computer*: CRAY-1; *Installation*: SRC, Daresbury Laboratory, Warrington.

*Operating system*: COS 1.09

*Programming language used*: ANSI FORTRAN 66

*High speed storage required*: 354 595 words

*No. of bits in a word*: 64

*Overlay structure*: none

*No. of magnetic tapes required*: 2 or 3

*Other peripherals used*: card reader, lineprinter, scratch disc store, permanent disc store

*No. of cards in source program*: 9546

*eference to other published version of this program*:

*atalogue number*: AAHH

*tle*: A new version of RMATRX STG3

*ef. in CPC*: 14 (1978) 367

*PC Library subprograms used*:

*atalogue numbers*: AANR, AANS, AANT, AANU

*tles*: RMATRX STG1R, RMATRX STG2R, RMATRX RE-
UP, RMATRX RECUD

*ef. in CPC*: this paper

*eywords*: atomic, electron–atom, scattering, electron–ion, otoionization, *R*-matrix, Breit–Pauli Hamiltonian, House-
lder method, eigenvalues, eigenvectors, cross-sections, Buttle
rrection, De Vogelaere's method, phase shift, *K*-matrix, *T*-
atrix, relativistic effects, fine structure levels, coupled dif-
rential equations

*ature of the physical problem*

his program reads the Hamiltonian matrix, the asymptotic potential coefficients and dipole length and velocity matrices. If the calculation is in *LS*-coupling these have been calculated in RMATRX STG2R [1]. If relativistic effects are included and cross sections between fine structure levels required they will have been calculated in RMATRX RECUP and RMATRX RECUD [1]. The code then diagonalizes the Hamiltonian matrix and calculates the *R*-matrix and its Buttle correction. Then either the electron–atom or electron–ion cross section, the photoionization cross section or $\beta$ parameter is calculated for a range of incident energies or frequencies.

*Restrictions on the complexity of the program*

Consult subroutine SETDIM of RMATRX STG3R to determine the current dimensions.

*Typical running time*

The dominating factor is the number of channels and the time taken to solve the coupled differential equations. The test run took 30 s on a CRAY-1.

*Reference*

[1] N.S. Scott and K.T. Taylor, this paper.

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Computer Physics Communications 25 (1982) 389–416
North-Holland Publishing Company

# CALCULATION OF THE IMPACT SCATTERING CONTRIBUTION TO ELECTRON ENERGY LOSS SPECTRA

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*Science Research Council, Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK*

Received 23 November 1981

## PROGRAM SUMMARY

*Title of program*: EELSOV

*Catalogue No.*: AARU

*Computer*: IBM 370/165, CRAY-1; *Installation*: Daresbury Laboratory

*Operating system*: OS, COS

*Programming language*: FORTRAN IV (IBM)

*High speed storage required*: 300 Kbytes (IBM)

*No. of bits per word*: 32, 64

*Overlay structure*: none

*Peripherals used*: none

*No. of cards in program and test deck*: 4263

*Keywords*: electron energy loss spectroscopy, impact scattering, solid state, crystal, overlayer, surface, surface vibrations, surface phonons, multiple scattering

*Nature of the physical problem*
To calculate the impact scattering contribution to the electron energy loss current, from one or more adsorbate layers on a single crystal surface, as a function of vibrational frequency and polarisation, incident electron energy and direction and scattered electron direction.

*Method of solution*
Assuming the initial and final state energies to be the same, the energy loss matrix element is calculated to first order in the adsorbate displacement, and in the rigid muffin-tin approximation, for a simple harmonic surface vibration of given amplitude and polarisation. The initial and final state wavefunctions are calculated with full multiple scattering for one or more adsorbate layers, on a crystal described by sufficient identical layers to obtain the bulk reflectivity.

*Restrictions on the complexity of the problem*
1) The program assumes only one atom per unit cell in any given layer and that the bulk crystal is composed of identical layers.
2) Each layer including the adsorbate must be a sublattice of the layer below. This is of course satisfied by the bulk crystal layers.
3) The surface barrier is assumed to refract but not to reflect electrons. This assumption becomes poorer as the incident electron energy is lowered.
4) The dipole interaction is neglected. This program will only give a small part of the total current near the specular direction for modes of vibration perpendicular to the surface.
5) The incident and scattered electrons are assumed to have the same energy. This is reasonable for many systems where the phonon frequency is typically ≈ 100 meV compared to incident electron energies of a few eV.
6) Degenerate modes parallel to the surface must be treated with care since the program assumes a non-degenerate vibration with a well defined polarisation vector as the source of a particular loss peak. For vibrating atoms in two-fold sites e.g. W(100)p(1 × 1)H, where degenerate vibrations occur on separate sites, the total result for a parallel mode can be obtained for all angles by adding the intensities obtained from two possible sites. For atoms in four-fold sites e.g. Ni(100)p(1 × 1)CO, where degenerate vibrations occur on the same site, only scattering angles in the plane of incidence can be considered and for the scattering plane lying parallel to one direction of vibration. In this case the contribution to the current from vibrations perpendicular to the plane of incidence is zero.

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Computer Physics Communications 25 (1982) 417–431
North-Holland Publishing Company

# A SPECTRUM DATA PROCESSING SYSTEM

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*Dept. of Physics, Chalmers University of Technology, S-412 96 Göteborg, Sweden*

Received 26 November 1981

## PROGRAM SUMMARY

*Title of program:* MONIT

*Catalogue number:* AARV

*Computer:* HP1000; *Installation:* Dept. of Physics, Chalmers Univ. of Tech.

*Operating system:* RTE IV B

*Programming language used:* HP FORTRAN IV

*High speed storage required:* 24 Kwords (segments need another 42 K), see also introduction

*No. of bits in a word:* 16

*Overlay structure:* 11 segments

*No. of magnetic tapes required:* one (optional)

*Other peripherals used:* magnetic disc

*No. of cards in combined program and test deck:* 11769

*Keywords:* Auger, monitor system, spectroscopy

*Nature of physical problem*
This paper presents a program system intended for the collection and processing of spectrum data. The programs have been developed to be used with a minicomputer connected on-line to a spectrometer. The prime goal of the work has been to produce a user oriented system which could also be used by people unfamiliar with computer programming. With this system, data can be obtained and stored on disc files and easy magnetic tape back-up can be done. Furthermore, various types of spectrum manipulation are possible, such as smoothing, simple background reduction and peak fitting.

The program system has been developed for the handling of data from an Auger electron spectrometer. Only very few routines are, however, restricted in their use to Auger spectroscopy, so that this system could be useful in any physical experiment where data is collected in spectrum form.

*Method of solution*
The main program of the system is written as a monitor program in that it is capable of executing two-letter mnemonic commands. With this system, spectra can be obtained from the spectrometer and stored on a magnetic disc together with a comment about the content of the spectrum file. Furthermore, the system keeps a library of all spectrum files on the disc. The file names are entered into the library in alphabetic order. To enable quick transfer of disc files to a mass storage, the system provides an automatic disc/tape transfer facility. A directory of the magnetic tape files is kept on the magnetic tape itself, thus enabling easy transfer of files from the tape back to the disc.

Various routines for spectrum manipulation are included. Examples are: smoothing of spectra, simple background reduction and peak fitting. The last feature uses a fitting routine by Von Meerwall [1]. Peak parameters (position height and width) can be stored on disc files and a separate library of these files is also kept.

Sequences of commands can be executed via a learn-mode facility. These command sequences are stored in disc files and a third library is also kept for such files.

Using a Tektronix graphics terminal the spectra can be easily displayed and magnified to suite the needs of the operator. To simplify the use of the program system to untrained users, a "Help-program" can be called to give specific information about all the possible commands.

*Reference*
E. von Meerwall, Comput. Phys. Commun. 9 (1975) 117.

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Computer Physics Communications 25 (1982) 433–436
North-Holland Publishing Company

# POSDIF – A PROGRAM TO COMPUTE POSITRON DIFFUSION AND ANNIHILATION IN RARE GASES

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Received 24 November 1981

## PROGRAM SUMMARY

*Title of program:* POSDIF

*Catalogue number:* AAHN

*Computer:* IBM-360 at York University, Toronto and also CDC 7600 at ULCC, University of London and Felix C-256 at University of Cluj Computer Centre.

*Programming language used:* FORTRAN IV

*Storage required:* 26 kwords in double precision

*Number of bits in a word:* 32

*Overlay structure:* none

*Peripherals used:* card reader, line printer

*Number of cards in the program and the test deck:* 917

*Keywords:* positron, diffusion equation, lifetime spectrum, Crank–Nicolson method, finite differences, momentum transfer, effective charge

*Nature of the physical problem*
Calculates positron lifetime spectrum in a gas being given the gas pressure and temperature, the value of the external electric field strength and the fits to momentum dependence of the positron–atom momentum transfer cross section and of the effective charge number [1].

*Method of solution*
The parabolic equation, representing positron diffusion and annihilation in the gas, is solved using the Crank–Nicholson method and other standard finite difference methods [2]. At each timestep the velocity distribution is used to calculate the averaged effective charge number and the averaged positron momentum.

*Typical running time*
About 300 s CPU time on the IBM-360.

## References

[1] R.I. Câmpeanu and J.W. Humberston, J, Phys. B 10 (1977) 239.
[2] Harwell Subroutine Library, Report AERE-R9185, HMSO London (September 1980).

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Computer Physics Communications 27 (1982) 25–37
North-Holland Publishing Company

# A NEW PROGRAM TO CALCULATE DIFFERENTIAL AND TOTAL CROSS SECTIONS FOR ELECTRON–ATOM OR ION SCATTERING USING THE MOMENTUM TRANSFER FORMALISM

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Received 16 November 1981

## PROGRAM SUMMARY

*Title of program:* MOMTRANF

*Catalogue number:* AANW

*Computer*: AS/7000; *Installation:* Daresbury Laboratory

*Operating system:* HASP

*Program language used:* FORTRAN IV

*High speed storage required:* 200 Kbytes

*Number of bits in a word:* 64

*Overlay structure:* none

Peripherals used: depending on the options used, generally none

*Number of cards in combined program and test deck:* 2590

*Keywords:* atomic, ionic, molecular, differential cross section, total cross section, momentum transfer, excitation, rotation, vibration

*Nature of physcial problem*
The scattering of low energy electrons by atoms or ions in the *LS* coupling scheme, or the rotational or roto-vibrational excitation of diatomic molecules by electron impact in the laboratory frame.

*Typical running time*
.26 s for test run I.

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Computer Physics Communications 27 (1982) 39–48
North-Holland Publishing Company

# MULTIQUARK CALCULATIONS WITH SCHOONSCHIP

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Received 18 June 1981, in revised form 18 January 1982

## PROGRAM SUMMARY

*Title of program:* MULTIQUARK (collection of SCHOONSCHIP-BLOCKS) plus two test programs PSIGEN and HCMPSI showing the use of these BLOCKS

*Catalogue number:* AAVG

*Computer:* CDC Cyber 70-74; *Installation:* RBK Computer Centre, University of Oslo

*Programming language used:* SCHOONSCHIP

*Operating system:* NOS/BE level 473

*High speed storage required:* 64 K

*Number of bits in a word:* 60

*Overlay structure:* none

*Peripherals used:* 1 disk pack and 1 line printer

*Number of cards in combined program and test deck:* 1038

*Keywords:* multiquark spectroscopy, colour-magnetic interaction, broken flavour symmetry, construction of wavefunctions in colour-, flavour- and spin-space

*Nature of the physical problem*
The purpose of MULTIQUARK is to use the algebra program SCHOONSCHIP to calculate the spectrum of multiquark systems. For this purpose the colour-magnetic interaction $H_{\mathrm{CM}}$ has to be found. It is shown how this operator can be programmed in SCHOONSCHIP using the substitution facility.

*Method of solution*
The highest states in colour, spin and flavour space of the irreducible representations that can possibly be mixed under the action of $H_{\mathrm{CM}}$ have to be present when the program starts. The problem is then solved in two steps. The first step is to create the wavefunctions we are interested in. These are created from the highest states using step-operators in colour-, spin- and flavour-space. The necessary step operators are included among the BLOCKS (equivalent to subroutines in FORTRAN). These wavefunctions, declared as COMMON variables, will be present on TAPE5 at the end of the program. These wavefunctions are used as input to the second program, where $H_{\mathrm{CM}}$ is applied to one of the wavefunctions.

*estrictions on the complexity of the problem*

he problem worked out in detail here is for $4q\bar{q}$ systems. It is therefore easily also used for any subgroup of quarks present in this ystem, for instance qqq or $q\bar{q}$. If one wants to increase the number of quarks beyond $4q\bar{q}$ the methods employed here are easily eneralized.

*eference*

1] H. Strubbe, Comput. Phys. Commun. 8 (1974) 1.

Computer Physics Communications 27 (1982) 49–55
North-Holland Publishing Company

# PROVA, A PROGRAM FOR THE CALCULATION OF X-RAY POWDER SPECTRA (ORDERED AND DISORDERED STRUCTURES)

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David AJÒ
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and Viscardo MALTA
*Centro di Studio per la Fisica delle Macromolecole del CNR, Bologna, Italy*

Received 22 April 1981; in revised form 14 January 1982

## PROGRAM SUMMARY

*Title of program:* PROVA

*Catalogue number:* AASE

*Computer:* CYBER 76; *Installation:* CINECA, Casalecchio di Reno, Bologna, Italy

*Operating system:* SCOPE 2.1

*Programming language used:* FORTRAN CDC

*High speed storage required:* 5936 words

*No. of bits in a word:* 60

*Overlay structure:* none

*Peripherals used:* card reader, line printer

*No. of cards in combined program and test deck:* 718

*Keywords:* crystallography, X-ray intensities, powder diffraction, disorder, stacking faults, crystal structure

*Nature of the physical problem*
PROVA calculates the X-ray intensity diffracted from powders constituted by generic domains, whatever the dimensions of each domain along the three crystallographic axes, possibly disordered, having unit cells belonging to any crystal system.

*Method of solution*
The calculation of the powder X-ray intensity requires the evaluation of one surface integral for each point of the calculated spectrum. In PROVA, the integration is performed by the Gauss method.

*Restrictions on the complexity of the problem*
The program can deal only with parallelepiped-shaped domains. In the present version only unidimensional disorder can be taken into account.

*Unusual features of the program*
Hollerith strings are delimited by stars. The first statement (PROGRAM...) is peculiar to the CDC systems.

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Computer Physics Communications 27 (1982) 57–64
North-Holland Publishing Company

# NUMBER OF REPRESENTATIONS AND MAXIMUM DIMENSIONS FOR S(N)

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and R. MIRMAN
*155 E 34 St., New York, NY 10016, USA*

Received 16 November 1981

## PROGRAM SUMMARY

*Title of program:* SYMBNDS

*Catalogue number:* AAMI

*Computer:* IBM 3033: *Installation:* City University of New York-University Computer Center

*Operating system:* OS/MVS/JES3

*Programming language used:* PL/I Optimizer

*High speed storage required:* 130 kbytes through S(30)

*No. of bits in a byte:* 8

*Overlay structure:* none

*Peripherals used:* card reader, line printer, card punch or terminal

*No. of cards in combined program and test deck:* 182

*CPC library subprograms for which this program is used:*

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAMC | SYMGRPTB | 23 (1981) 81 |
| AAMD | NGHBTRNS | 23 (1981) 81 |
| AAME | SYMSTATS | 23 (1981) 95 |
| AAMF | SYMRPMAT | 23 (1981) 95 |

*Keywords:* general purpose, symmetric group, number of representations, maximum dimension

*Nature of the physical problem*
To find the number of representations of each symmetric group, and a bound on the maximum dimension of the representations for each symmetric group.

*Method of solution*
Use expressions giving required values.

*Restrictions on the size of the problem*
Can be used for any symmetric group for which machine time and storage are available.

*Typical running times*
Through S(30): 1.42 s.

Computer Physics Communications 27 (1982) 65–71
North-Holland Publishing Company

# PROION: A CODE FOR CALCULATING IONISATION THRESHOLD INTENSITIES AND IONISATION PERIODS IN HIGH-INTENSITY-LASER IRRADIATED PLASMAS

B.W. BOREHAM *

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Received 19 December 1980; in final form 29 January 1982

## PROGRAM SUMMARY

*Title of program:* PROION

*Catalogue Number:* AARY

*Computer:* UNIVAC 1108 and 1100/42; *Installation:* Australian National University, Canberra **

*Operating system:* EXEC – 8

*Programming language used:* FORTRAN

*High speed store required:* 373248 words

*Number of bits in a word:* 36

*Overlay structure:* none

*Peripherals used:* line printer, card reader

*Number of cards in combined program and test deck:* version 1: 176, version 2: 205

*Keywords:* ionisation, laser, ionisation probability function, high intensity, tunneling

*Nature of the physical problem*
The evaluation of ionisation threshold intensities (the minimum intensity at which ionisation will occur) and the ionisation period for irradiation of the test gas with intensities greater than the threshold intensities.

*Method of solution*
PROION calculates ionisation intensities and ionisation periods using the general theory of ionisation of Keldysh [1]. The ionisation threshold intensity or ionisation period and intensity at which ionisation occurs for intensities greater than the threshold, are calculated by iteration using the Keldysh ionisation probability function for the input ionisation potential of the test gas, the laser beam minimum intensity and the laser beam pulse width.

*Restrictions on the complexity of the problem*
The calculation is restricted to the tunneling limit (strong field) case of the Keldysh general formula, although the program can be easily adapted to the other limiting case of multiphoton absorption (moderate electric fields). The calculation is restricted further to exclude Coulomb force corrections, since it is this case that agrees best with experiment [2].

The laser wavelength is assumed to be 1.06 $\mu$m, but the calculation is not strongly dependent on wavelength and may be readily adapted for lasers other than neodymium.

*Unusual features of the program*
PROION is in standard FORTRAN except for the input lists, which are in free format.

*References*

[1] L.V. Keldysh, Sov. Phys. JETP 20 (1966) 1307.
[2] B.W. Boreham, Europhysics Study Conf. on Multiphoton Processes, Bénodet, France (18–22 June 1979).

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** Now also available on a CDC Cyber 174/6500 system located at Imperial College. CDC operation requires an additional program card. For UNIVAC operation this card (the first executable statement) must be removed.

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North-Holland Publishing Company

# NEWTON–EVERETT INTERPOLATION OF CONTINUOUS FUNCTIONS

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Received 3 November 1981

## PROGRAM SUMMARY

*Title of program*: FINT

*Catalogue number*: AARS

*Computer*: IBM 370/158; *Installation*: Comisión Nacional de Energía Atómica, Av. del Libertador 8250, 1429 Buenos Aires, Argentina

*Operating system*: OS/VS1 or VM370/CMS

*Programming language used*: FORTRAN IV

*High speed storage required*: 234 Kbytes

*No. of bits in a word*: 32

*Overlay structure*: none

*No. of magnetic tapes required*: none

*No. of cards in combined program and test deck*: 673

*Keywords*: general purpose, Newton interpolation, Everett interpolation, finite differences, continuous approximation

*Nature of physical problem*

Interpolation needs are deeply rooted in almost all branches of physics because of the uncommonness of analytical solutions and the discrete nature of physical measurements.

*Method of solution*

If the calculations one is doing are very time consuming, it would be convenient to minimize these calculations and to interpolate whenever possible. In this paper we describe an interpolation routine that employs the finite difference formulae of Newton and Everett [1].

The routine is designed to work with a continuous function defined on an evenly spaced set of points. The main purpose is to do the calculations in a quick and accurate form. The calculation is divided into two parts:

i) a calculation which depends exclusively on the points where the function is given and on the accuracy requested;

ii) a calculation dependent on the point where one wishes to interpolate.

The first calculations are done only once and are then available for the following calculations.

*Restrictions on the complexity of the program*

In the program it is assumed that the set of points where the function is defined is less than or equal to 200. This can be easily changed.

If the function to be interpolated has a pathological behaviour, the results are strongly dependent on the size of the separation between functional values, so special care must be taken with this point (see section 3).

*Typical running time*

The average running time depends on the number of interpolation points calculated. However, it can be estimated to be of the order of 3 times that needed for a double-precision exponential (see section 3).

*Reference*

[1] Z. Kopal, Numerical analysis (Chapman and Hall, London, 1961).

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Computer Physics Communications 27 (1982) 79–86
North-Holland Publishing Company

# MATSUP: A PROGRAM TO OBTAIN TWO-ELECTRON REPULSION INTEGRALS FROM A SPARSE FILE OF $\mathcal{P}$ SUPERMATRIX ELEMENTS

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Received 18 May 1981

## PROGRAM SUMMARY

*Title of program*: MATSUP

*Catalogue number*: AARZ

*Computer*: UNIVAC 1110; *Installation*: Centre de Calcul de Strasbourg-Cronenbourg, rue du Loess, 67000 Strasbourg, France

*Operating system*: EXEC 8

*Programming language used*: FORTRAN IV

*High speed storage required*: 31280 words

*No. of bits in a word*: 36

*Overlay structure*: none

*No. of magnetic tapes required*: 2

*Other peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 840

*Program limitation*: the storage requirement presented here corresponds to a maximum number of 150 contracted Gaussians in the basis set

*Specific library routines*:

i) DEFINE IDUM=FLD (IBIT1, NSTR, WORD)
This function defines a string of NSTR bits starting at bit number IBIT1 in the dummy variable WORD. The DEFINE statement is written before any executable statement. In the program, the function can be used either to enter the bit string into a variable:
IDUM=I
VAR=WORD
or to retrieve the bit string from a variable:
WORD=VAR
I=IDUM
If WORD has to be partitioned into several strings, each string must be defined with a specific DEFINE statement.

ii) CALL IOW (IFILE,IOP,N,A(1),K,ISTAT)
is a local library routine transferring N words starting from address A(1) to – or from – IFILE. The flag ISTAT checks the I/O operation. For the user, this routine is equivalent to a nonformatted READ/WRITE statement.

iii) MULTAP (IFILE) is a library routine designed to manage the multivolume files.

iv) Time routines TDELTA (SUP time) and FDELTA (CPU time).

*Keywords*: conversion, integrals, electron repulsion, supermatrix

*Nature of the physical problem*
The iterative resolution of the Roothaan equations in the SCF procedure [1] can be carried out either from the file of two-electron repulsion integrals $(pq|rs)$, or from a file of supermatrix elements, defined as

$$\mathcal{P}_{pq,rs}=(pq|rs)-\tfrac{1}{4}[(pr|qs)+(ps|qr)]. \qquad (1)$$

The iterative cycles are intrinsically faster when carried out from the $\mathcal{P}$ supermatrix file [2]. However, the file of two-electron repulsion integrals is requested when the wavefunction is improved beyond the Hartree–Fock approximation, by means of configuration interaction. Therefore, there is a clear need for a program designed to convert efficiently a $\mathcal{P}$ supermatrix file into a classical file of two-electron repulsion integrals.

### *Method of solution*

If the file of $\mathcal{P}$ supermatrix elements is assumed to be complete the conversion is performed through a system of three relations involving the elements of $\mathcal{P}$ obtained from the three nonequivalent permutations of indices $p$, $q$, $r$, $s$ (assuming $p > q > r > s$).

$$\begin{aligned}(pq|rs)&=1.2\mathcal{P}_{pq,rs}+0.4\left[\mathcal{P}_{pr,qs}+\mathcal{P}_{ps,qr}\right],\\(pr|qs)&=1.2\mathcal{P}_{pr,qs}+0.4\left[\mathcal{P}_{pq,rs}+\mathcal{P}_{ps,qr}\right],\\(ps|qr)&=1.2\mathcal{P}_{ps,qr}+0.4\left[\mathcal{P}_{pq,rs}+\mathcal{P}_{pr,qs}\right].\end{aligned} \tag{2}$$

This relationship defines a "set" of integrals.

If some of these indices are coincident (cases $p = q$; $q = r$; $r = s$ and combinations), the size of the set is reduced from 3 to either 2 or 1. Each case is analyzed and processed separately. However, a real $\mathcal{P}$ file is usually not complete, but sparse. It means that some of the nonequivalent $\mathcal{P}$ elements are omitted in the file either because they are zero by symmetry or because they are lower than a given threshold. For each set of $\mathcal{P}$ elements, the presence of such "holes" is detected by the program. In the frame of either relation system (2) or its convenient subset, a value of zero is assigned to the deleted permutations of $\mathcal{P}_{pq,rs}$. Therefore in an intermediate step, a complete set of two-electron integrals is obtained from a set of $\mathcal{P}$ elements which may be noncomplete. Then the obtained integrals are checked against a threshold and either kept or deleted.

### *Typical running time*

About 210 s for 1 million $\mathcal{P}$ elements.

### *References*

[1] C.C.J. Roothaan, Rev. Mod. Phys. 23 (1951) 69.

[2] See for instance A. Veillard, in: Computational techniques in quantum chemistry and molecular physics (Reidel, Dordrecht, 1975) p. 201.

Computer Physics Communications 27 (1982) 129–146
North-Holland Publishing Company

# VMOMS – A COMPUTER CODE FOR FINDING MOMENT SOLUTIONS TO THE GRAD–SHAFRÁNOV EQUATION *

L.L. LAO †, R.M. WIELAND, W.A. HOULBERG and S.P. HIRSHMAN

*Oak Ridge National Laboratory, Oak Ridge, TN37830, USA*

Received 7 December 1981

## PROGRAM SUMMARY

*Title of program*: VMOMS

*Catalogue number*: ABSH

*Computer*: PDP-10/KL10; *Installation*: ORNL Fusion Energy Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA

*Operating system*: TOPS 10

*Programming language used*: FORTRAN

*High speed storage required*: 9000 words

*No. of bits in a word*: 36

*Overlay structure*: none

*Peripherals used*: line printer, disk drive

*No. of cards in combined program and test deck*: 2839

*Keywords*: plasma physics, variational principle, Grad–Shafranov equation, moments, shooting method

*Nature of the physical problem*
This code finds approximate solutions to the Grad–Shafranov equation describing scalar pressure-balance equilibria for axisymmetric tokamak plasmas. A Fourier series expansion of the flux surface coordinates $(R, Z)$ is made in terms of two new coordinates $(\rho, \theta)$, and the resulting equation is conveniently reduced to a system of ordinary differential equations (ODE's) using a variational principle [1]. The solution of these simple equations with pressure and current as driving functions yields, in principle, a complete description of the equilibrium.

*Method of solution*
The system of ODE's is solved numerically by a shooting method using D02AGF, a suite of subroutines in the NAG library [2].

*Restrictions on the complexity of the problem*
Complete axisymmetry is assumed, as well as up–down symmetry about the toroidal midplane.

*Unusual features of the program*
VMOMS uses a suite of routines D02AGF developed by I. Gladwell and available from the NAG library [2] of mathematical software. An annotated version of these routines is included in the source file. A data file is generated for easy postprocessing of the results and subsequent plotting. A plotting routine, adapted for use on the DEC PDP-10, has been included as a guide to generating the plots.

*References*

[1] L.L. Lao, S.P. Hirshman and R.M. Wieland, Phys. Fluids 24 (1981) 1431.
[2] Numerical Algorithms Group (NAG) Library Manual, Mark 8 (1981).

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* Research sponsored by the Office of Fusion Energy, US Department of Energy, under contract W-7405-eng-26 with the Union Carbide Corporation.

† Current address: General Atomic Co., San Diego, CA 92138, USA.

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Computer Physics Communications 27 (1982) 147–166
North-Holland Publishing Company

# COULFG: COULOMB AND BESSEL FUNCTIONS AND THEIR DERIVATIVES, FOR REAL ARGUMENTS, BY STEED'S METHOD

A.R. BARNETT

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Received 15 December 1981

## PROGRAM SUMMARY

*Title of program*: COULFG: Coulomb, Bessel Functions

*Catalogue number*: ABNK

*Computer*: IBM 370/165 and AS/7000; *Installation*: Daresbury Laboratory, Warrington, Lancs.

*Operating system*: OS/360 GI compiler and HX compiler (level 2.2.1)

*Programming language used*: ASA FORTRAN

*High speed storage required*: 180 Kbytes

*No. of bits in a word*: 32

*Overlay structure*: none

*Peripherals used*: card reader, printer

*No. of cards in combined program and test deck*: 432

*Keywords*: Klein–Gordon, Coulomb for real angular momentum, recurrence relations, Schrödinger, Bessel, spherical Bessel, continued fraction, reactions, scattering, heavy ion, nuclear, molecular, atomic, pionic, kaonic, exotic atoms, scattering states

*Nature of physical problem*
Coulomb interaction of charged particles in spherical coordinates (Coulomb function) and uncharged particles (spherical Bessel functions), and general problems in cylindrical coordinates yielding Bessel-function solutions can be solved with the program. COULFG computes the Coulomb wavefunctions $F_\lambda(\eta, x)$, $G_\lambda(\eta, x)$, $F'_\lambda(\eta, x)$ and $G'_\lambda(\eta, x)$ for a range of $\lambda$-values in integer steps, $l \geqslant \lambda \geqslant m > -1$, for real $x > 0$ and real $\eta$, $10^4 \geqslant |\eta|$. Values of the maximum angular momentum, $l$, of several thousand can be treated. When the functions have oscillating character the absolute accuracies are about $10^{-14}$ but this is only limited by the word length used; extended precision variables can yield absolute accuracies of $10^{-30}$. COULFG will generate spherical Bessel functions and cylindrical Bessel functions for a wide range of integer-spaced real orders.

*Method of solution*
An enhanced version of Steed's method, used previously for integer $\lambda$ in subroutine RCWFN [1] is adopted. The more recent subroutine KLEIN [2] for a single $\lambda$ value also is similar, the additional feature being the stable recurrence relations for a range of $\lambda$ values.

*Restriction on the complexity of the problem*
It is well known that the method used loses accuracy as $x < x_m$ (the turning point for the minimum order required) and eventually, when $G_m \gtrsim 10^6$, a JWKB approximate solution is adopted which is accurate to $\lesssim 1\%$ as a rule. Several output variables signal that this has occurred.

*Features of the program*
A considerably revised version is presented of the CPC program 'RCWFN' (catalogue ABPC) used to compute the Coulomb functions $F_L(\eta, x,$ $G_L(\eta, x)$ and their $x$-derivatives over a range of integer $L$-values $\geqslant 0$. The new program, COULFG, calculates $F_\lambda(\eta, x)$, $G_\lambda(\eta, x)$, $F'_\lambda(\eta, x)$ and $G'_\lambda(\eta, x)$ when $\lambda$ is real ($\lambda > -1$) and for a similar range in the $(\eta, x)$ plane as before, $10^4 \geqslant x > 0$, $10^4 \geqslant |\eta|$. Integer-spaced $\lambda$-values are obtained by a suitable combination of stable recurrence relations. Subroutine COULFG will return, furthermore, for a range of integer-spaced orders;

a) Spherical Bessel functions $j_\lambda(x)$, $y_\lambda(x)$, $j'_\lambda(x)$, $y'_\lambda(x)$, and
b) Cylindrical Bessel functions $J_\mu(x)$, $Y_\mu(x)$, $J'_\mu(x)$, $Y'_\mu(x)$, where both $\lambda$, $\eta$ can be real or integral. Values of order in excess of 1000 have been tested.

A "mode" option is provided so that, for each case, arrays of the regular and irregular functions and their derivatives, or just the two functions, or the regular function alone ($F_\lambda$, $j_\lambda$, $J_\mu$) are calculated and stored. Both core and execution time are saved by this technique.

In the region of $x$ where the functions oscillate, i.e. $x \geqslant x_\lambda$ (the turning point for the λth partial wave) the relative accuracy of the functions for IBM machines (REAL∗8) as programmed, is $\approx 10^{-14}$–$10^{-16}$ and for CDC machines (single precision) is $\approx 10^{-12}$–$10^{-14}$. With no change in the code except for the accuracy parameter the accuracy can be increased to $\approx 10^{-30}$ by using the AUTODOUBLE facility on an extended-precision IBM compiler. The accuracy decreases in a predictable way as $x$ decreases below $x_\lambda$; a measure of this decreased accuracy is provided by the program. JWKB approximations are provided when $x$ is sufficiently smaller than $x_\lambda$.

*Typical running time*

The test deck ran in $2\frac{1}{2}$ s on the Gl compiler and the HX compiler, one half of which demonstrates error conditions.

*References*

[1] A.R. Barnett, D.H. Feng, J.W. Steed and L.J.B. Goldfarb, Comput. Phys. Commun. 8 (1974) 377.
[2] A.R. Barnett, Comput. Phys. Commun. 24 (1981) 141.

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Computer Physics Communications 27 (1982) 167–178
North-Holland Publishing Company

# TWO-DIMENSIONAL ADAPTIVE QUADRATURE OVER RECTANGULAR REGIONS

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Received 24 September 1981

## PROGRAM SUMMARY

*Title of program*: QADAPT

*Catalogue number*: AAZA

*Computer*: Sperry Univac 1100/82; *Installation*: Madison Academic Computer Center

*Operating system*: Exec 8

*Programming language*: FORTRAN 77

*High speed storage required*: variable; approx. 33000 words

*Number of bits in a word*: 36

*Overlay structure*: none

*Peripherals*: card reader, line printer

*Number of cards in combined program and test deck*: 1229

*Keywords*: integration, quadrature, adaptive, multidimensional, Richardson extrapolation, simplex

*Nature of the physical problem*
Program QADAPT estimates the integral $F$ of an arbitrary function $f(x, y)$ over the unit square:

$$F=\int_0^1\int_0^1 f(x,y)\,\mathrm{d}x\,\mathrm{d}y.$$

Any integral over a two-dimensional rectangular region may be written in this form. The value of $F$ is computed to a specified relative accuracy and an error estimate is returned.

*Method of calculation*
The program is an adaptation of the multidimensional algorithm developed by Kahaner and Wells [1]. A more cautious extrapolation procedure and an error estimate suggested by Ström [2] are used.

*Restrictions on the complexity of the problem*
The extrapolation procedures used are strictly valid only for analytic integrands. Nevertheless, the program is generally reliable even if this requirement is violated at a finite number of points. Integration of rapidly varying or highly oscillatory functions may require more table space than specified in the test deck.

*Running time*
Execution of the two test cases which accompany this paper took approximately 0.7 CPU s.

*Unusual features*
The program provides adaptive subdivision of the region of integration and variable quadrature order. A global error reduction strategy guides the computation. Function values are stored using a double hashing technique for efficient reuse.

*References*

[1] D.K. Kahaner and M.B. Wells, ACM Trans. Math. Software 5 (1979) 86.
[2] T. Ström, BIT 13 (1973) 196.

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* Present address: Shell Development Co., P.O. Box 1380, Houston, TX 77001, USA.

Computer Physics Communications 27 (1982) 179–186
North-Holland Publishing Company

# A REDUCE PACKAGE FOR DETERMINING LIE SYMMETRIES OF ORDINARY AND PARTIAL DIFFERENTIAL EQUATIONS

Fritz SCHWARZ

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Received 1 September 1981; in final form 10 March 1982

## PROGRAM SUMMARY

*Title of programs*: LIE0,LIE1,LIE2,LIE3,LIE4

*Catalogue number*: AAZB

*Computer*: Siemens 7.760

*Operating system*: BS 2000

*Programming language used*: LISP

*High speed storage required*: depends on the problem, minimum about 400000 bytes

*No. of bits in a word*: 32

*Number of cards in combined program and test deck*: 200

*Keywords*: Ordinary differential equations, partial differential equations, Lie symmetries

*Nature of physical problem*
Lie symmetries of differential equations play an important role in all branches of physics. Usually they have a physical meaning. To know all Lie symmetries for a given problem is therefore of utmost importance because it usually leads to additional physical insight.

*Restrictions on the complexity of the problem*
In most cases the available computer memory is the severest restriction. It may only be avoided if the problem is split into several smaller ones.

*Running time*
It depends heavily on the number of dependent and independent variables and the structure of the problem. It cannot be estimated in advance.

Computer Physics Communications 27 (1982) 187–199
North-Holland Publishing Company

# PROGRAM FOR *B*-SPLINE INTERPOLATION OF SURFACES WITH APPLICATION TO COMPUTER TOMOGRAPHY *

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Received 1 September 1981; in final form 7 April 1982

## PROGRAM SUMMARY

*Title of program*: RAMFLA

*Catalogue number:* AARO

*Computer*: VAX 11 Digital; *Installation*: D.K.F.Z. Heidelberg

*Operating system*: VAX/VMS

*Programming language used*: FORTRAN 77

*High speed storage required*: greater than 256×256, depends on the user choice for the number of surface elements

*No. of bits in a word:* 32

*Overlay structure*: none

*Peripherals used*: TEKTRONIX display, RAMTEK color display

*No. of cards in combined program and test deck*: 3618

*Keywords*: computer tomography, *B*-spline interpolation, parametrically defined surfaces, computer graphics for intersections between straight lines, planes and surfaces, visible surface plot, surface shadowing

*Nature of physical problem and method of solution*
The interactive package presented here is used to interpolate by a nine-point formula a general surface given by the equation:

$F(X, Y, Z)=0$

with the arguments parametrically defined by:

$X=f(u, v)$: $Y=g(u, v)$; $Z=h(u, v)$.

Use is made of 3 bicubic (or biparabolic or bilinear) *B*-splines in order to interpolate $f$, $g$ and $h$, respectively. The main application is the reconstruction of surfaces given in computer tomography. Hidden lines are deleted, and a shadowed program is also provided.

*Restriction of the complexity of the problem*
The interpolation points must be provided in a set of non-intersecting contours.

*Typical running time*
Depends on the number of interpolation points, particularly for the hidden point process.

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* Dedicated to Professor K.E. Scheer for his 60th birthday.

Computer Physics Communications 27 (1982) 201–212
North-Holland Publishing Company

# UNIMOL: A PROGRAM FOR MONTE CARLO SIMULATION OF RRKM UNIMOLECULAR DECOMPOSITION IN MOLECULAR BEAM EXPERIMENTS

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Received 23 March 1982

## PROGRAM SUMMARY

*Title of program:* UNIMOL

*Cataloge number:* AAoA

*Computer:* IBM 3033N; *Installation:* Gothenburg Universities' Computing Centre

*Operating system:* OS MVS-SP1, JES2

*Programming language used:* FORTRAN

*High speed storage required:* 120832 words

*No. of bits in a word:* 32

*Overlay structure:* none

*Peripherals used:* card reader, line printer, card punch

*No. of cards in combined program and test deck:* 2222

*Keywords:* Unimolecular decomposition, RRKM-theory, transition state, centrifugal barrier, angular momentum conservation, reaction cross sections, branching ratio, Monte Carlo sampling

*Nature of the physical problem*

Reactive and nonreactive absolute angular distributions are measured in crossed molecular beam experiments. Absolute cross sections and branching ratios can be determined in the experiment only with some form of simulation algorithm.

*Method of solution*

The procedure uses Monte Carlo techniques to simulate the formation and decomposition of the complex. Angular momentum conservation, the simultaneous interaction of several decomposition channels and strict flux conservation are included in the procedure. Three nonstatistical effects, based on trajectory calculations and dynamical arguments, are also considered [1,2].

*Restrictions to the complexity of the problem*

Only three atomic complexes are considered.

*Typical running time*

Running time is almost proportional to the number of sampled systems. In the test run 80000 complex forming systems takes about seven minutes on the IBM 3033N.

*Unusual features of the program*

Three subroutines are used from the IMSL- and Harwell subroutine libraries.

*References*

[1] L. Holmlid and K. Rynefors, Chem. Phys. 60 (1981) 393.
[2] K. Rynefors and L. Holmlid, Chem. Phys. 60 (1981) 405.

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Computer Physics Communications 27 (1982) 229–242
North-Holland Publishing Company

# CONTIN: A GENERAL PURPOSE CONSTRAINED REGULARIZATION PROGRAM FOR INVERTING NOISY LINEAR ALGEBRAIC AND INTEGRAL EQUATIONS

Stephen W. PROVENCHER

*EMBL, Postfach 10.2209, D-6900 Heidelberg, Fed. Rep. Germany*

Received 5 May 1982

## PROGRAM SUMMARY

*Title of program*: CONTIN

*Catalogue number*: AAOB (version 2DP), AAOC (version 2 SP)

*Computer*: VAX 11/780; *Installation*: European Molecular Biology Laboratory (EMBL). The program is intended to be fully portable. After setting four installation dependent values, it should run without modification on most systems supporting 1966 ANSI standard Fortran IV. Version 2SP is recommended for machines (e.g., CRAY or CDC) with Fortran REAL representations of at least 60 bits and Version 2DP for all other machines

*Operating system*: VMS

*Programming language used*: Fortran IV (1966 ANSI standard, except for 1 in the rightmost DIMENSION specification of some dummy arrays)

*High speed storage required*: about 200 kbytes (depending on the size of the problem)

*No. of bits in a byte*: 8

*Overlay structure*: none

*No. of cards in combined program and test deck*: 5822

*Keywords*: regularization, inequality constraints, ill-posed, inverse problems, integral equations, quadratic programming, deconvolution, information content, superresolution, photon correlation, constrained least squares

*Nature of the physical problem*
Many experiments are indirect in that the observed data are linear integral (or matrix) transforms of the quantities to be estimated. These transforms typically arise because of the imperfect impulse response of the detection system or because of the indirect nature of the experiment itself (as with Fourier transforms in diffraction and Laplace transforms in relaxation experiments). The inversion of these linear operator equations are generally ill-posed problems in that there exists a large number of possible solutions (with arbitrarily large deviations from each other) all of which fit the data to within experimental error. Therefore straightforward inversion procedures cannot be used and statistical regularization techniques are necessary.

*Method of solution*
A general purpose constrained regularization method [1] finds the simplest (most parsimonious) solution that is consistent with prior knowledge and the experimental data. The problem is formulated as a weighted least squares problem with an added quadratic form, the regularizor, which imposes parsimony (typically smoothness) or statistical prior knowledge. Numerically stable orthogonal decomposition and quadratic programming algorithms [2] are used to obtain the unique global solution subject to any linear equality or inequality constraints imposed by prior knowledge (e.g., nonnegativity). The regularization parameter can be automatically chosen on the basis of an *F*-test and confidence regions.

*Restrictions on the complexity of the problem*
Part of the computation time is proportional to the cube of the number of parameters used to represent the solution. Computations with no more than about 100 parameters can be done economically. This is usually more than adequate for solutions in one dimension, but not for two- or three-dimensional solutions.

*Unusual features of the program*

CONTIN has been designed to be easily adaptable to a wide variety of problems, but still easy to use. It consists of a fixed core of 53 subprograms plus 13 simple and thoroughly documented "USER" subprograms that define nearly all aspects of the problem. These USER subprograms usually do not have to be changed, but they can be easily modified to define nonstandard integral equations, data preprocessing, simulations, constraints, regularizors, statistical weighting, output, etc.

*References*

[1] S.W. Provencher, Comput. Phys. Commun. 27 (1982) 213.
[2] C.L. Lawson and R.J. Hanson, Solving Least Squares Problems (Prentice-Hall, Englewood Cliffs, 1974).

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Computer Physics Communications 27 (1982) 243–284
North-Holland Publishing Company

# THE LUND MONTE CARLO FOR JET FRAGMENTATION

Torbjörn SJÖSTRAND

*Department of Theoretical Physics, University of Lund, Sölvegatan 14A, S-223 62 Lund, Sweden*

Received 4 April 1982

## PROGRAM SUMMARY

*Title of program*: JETSET 4.3 G

*Catalogue number*: AAVJ

*Computer for which the program is designed and others on which it is operable*: ND, Univac, CDC and others with a FORTRAN 77 compiler

*Computer*: ND-50; *Installation*: University of Lund, Lund, Sweden

*Operating system*: SINTRAN III/VS

*Programming language used*: FORTRAN 77

*High speed storage required*: 28 Kwords

*No. of bits in word*: 32

*Overlay structure*: none

*Peripherals used*: terminal or card reader for input, terminal or line printer for output

*No. of cards in combined program and test deck*: 1987

*Keywords*: jet fragmentation, hadronization, quark jet, gluon jet, multiparticle production, Monte Carlo simulation

*Nature of physical problem*

In high energy collisions normally most of the particles in the final state appear within a few rather narrow cones. Each of these collections of particles, called jets, are assumed to be coming from the hadronization of an outgoing quark or gluon. QCD, the candidate theory of strong interactions, can be used perturbatively to describe the scattering or creation of these partons at small distance scales (high $Q^2$), and there are reasons to believe that the large distance behaviour of QCD makes quarks and gluons confined inside hadrons. Exactly how the confinement forces transform e.g. a quark into a jet of particles is, however, not known at present.

*Method of solution*

The Lund model provides a phenomenological description of hadronization. Colour charges are assumed to be connected by colour flux tubes, kinematically described by the massless relativistic string with no transverse excitations. A quark then corresponds to an endpoint on a string and a gluon to a kink on it. The breakup of these strings is described in an essentially iterative fashion, string → hadron + remainder-string, for fast particles corresponding to an iteration jet → hadron + remainder-jet, but at the same time providing a natural joining of the jets in the central region.

*Restrictions on the complexity of the problem*

Each string piece must have a certain minimum energy so as to be able to fragment into at least two particles. This corresponds to a minimum invariant mass between each two partons connected by a colour flux tube. Also, in the present implementation a jet system may contain at most ten connected partons and a total of at most 250 particles produced (including unstable particles which subsequently decay), but this is easily changed.

*Typical running time*

An event with a CM energy of 40 GeV and an average of 30 particles (of which 14 are charged) in the final state takes approximately 0.2 s. Generation time is roughly proportional to the multiplicity.

*Unusual features of the program*

A random number generator is required. Energy, momentum and flavour are conserved step by step in the fragmentation process.

Computer Physics Communications 27 (1982) 285–297
North-Holland Publishing Company

# SHAPE OF A POLYTROPIC PRIMARY

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Received 8 June 1981; in revised form 20 February 1982

## PROGRAM SUMMARY

*Title of program* BINARY

*Catalogue number*: AAEI

*Computer*: DEC2060; *Installation*: University of Saskatchewan

*Operating system*: TOPS-20

*Programming language used*: FORTRAN IV

*High speed storage required*: 44032 words

*No. of bits in a word*: 36

*Overlay structure*: none

*Peripheral used*: disc

*No. of cards in combined program and test deck*: 1915

*Keywords*: three-dimensional free-boundary problem, semidiscrete Galerkin method, structure, synchronous binary system

*Nature of the physical problem*
Computation of the shape of a polytropic primary in a binary system, especially the case when the separation distance is at its minimum [1].

*Method of solution*
The gravitational potential is expanded in terms of spherical harmonics and the coefficients in the truncated expansion, being functions of the radial coordinate, are then determined numerically.

*Restrictions*
(i) The polytropic index must not be smaller than one. This restriction comes from the numerical procedure and could be removed.
(ii) It is assumed that the shape and other structural details of the secondary do not appreciably influence the primary. This restricts the complexity of the program.

*Unusual features*

When solving the system of linear algebraic equations, the Gaussian elimination and the back substitution are executed in blocks and massive storage is used for storing and retrieving results of these operations. This feature of the program BINARY, unfortunately, decreases its portability.

*Reference*

[1] M.J. Miketinac and S.V. Parter, ZAMP 32 (1981) 204.

Computer Physics Communications 27 (1982) 299–307
North-Holland Publishing Company

# *R*-MATRIX PROPAGATION PROGRAM FOR SOLVING COUPLED SECOND-ORDER DIFFERENTIAL EQUATIONS

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and L.A. MORGAN

*Department of Statistics and Computer Science, Royal Holloway College, Egham, Surrey TW20 0EX, England*

Received 27 April 1982

## PROGRAM SUMMARY

*Title of program:* RPROP

*Catalogue number:* AAJK

*Computer:* NAS AS7000; *Installation:* SERC Daresbury Laboratory, Warrington, Cheshire, England

*Operating system:* MVT

*Programming language used:* FORTRAN IV

*High speed store required:* 24 Kwords for test case

*Number of bits in word:* 32 bits

*Overlay structure:* none

*Peripherals used:* card reader, line printer, scratch disc

*Number of cards in combined program and test desk:* 1508

*Keywords:* atomic, nuclear, *R*-matrix, scattering, electron–atom, electron–ion, electron–molecule, atom–molecule, asymptotic solution, differential equation, Hamiltonian matrix

*Nature of physical problem*
Coupled second-order differential equations which arise in electron collision with atoms, ions and molecules are solved over a given range of the independent variable. The *R*-matrix at one end of the range is calculated given the *R*-matrix at the other end of the range.

*Method of solution*
The range is divided into a number of subranges and the Hamiltonian is diagonalized in such subrange in terms of an expansion in shifted Legendre polynomials. A correction introduced by Bloch [1] is included at each end of each subrange. The integrals are carried out using Gauss–Legendre quadrature.

*Restrictions on the complexity of the problem*
The potential interaction is restricted to the long-range multipole potential between an electron and an atom ion or molecule. More general potentials, for example those occurring in atom–molecule scattering, could be treated by a straightforward modification of the program.

*Typical running times*
The program is most efficient if the calculation is required for many energy points in a limited range of energies. The time taken by the test run, which was inefficient since only one energy point was calculated, was 1.3 s.

*Reference*
[1] C. Bloch, Nucl. Phys. 4 (1957) 503.

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* Present address: University of Delhi, India.

** Also: Science & Engineering Research Council, Daresbury Laboratory, Warrington WA4 4AD, England.

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Computer Physics Communications 27 (1982) 309–322
North-Holland Publishing Company

# GAMOW, A PROGRAM FOR CALCULATING THE RESONANT STATE SOLUTION OF THE RADIAL SCHRÖDINGER EQUATION IN AN ARBITRARY OPTICAL POTENTIAL

T. VERTSE, K.F. PÁL and Z. BALOGH *

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Received 16 April 1982

## PROGRAM SUMMARY

*Title of program*: GAMOW FUNCTIONS

*Catalog number*: AAOD

*Computer*: ES-1040 (IBM 360 compatible); *Installation*: Hungarian Academy of Sciences Central Research Institute for Physics, Budapest, Hungary

*Operating system*: OS 28.F

*Other computers on which it is operable*: PDP 11, CDC 3300

*Programming language used*: FORTRAN IV

*High speed storage required*:
double precision version: 94 Kbytes,
single precision version: 76 Kbytes

*Number of bits per byte*: 8

*Overlay structure*: none

*Peripherals used*: line printer, card reader

*No. of cards in combined test deck*: 1359

*Keywords*: normalized Gamow functions, resonant states, single particle solution, Schrödinger equation, decaying states, complex eigen-solution, poles of scattering function, bound states in complex potential

*Nature of the physical problem*
The program calculates the normalized Gamow solution of the radial Schrödinger equation, i.e. the solution which is regular at the origin and has purely outgoing wave asymptotics, in a spherically symmetric complex potential of arbitrary form. Optionally either the complex energy eigenvalue in a given potential i.e. the position of the pole of the scattering function $S(E)$ or the strength of the short-range potential belonging to a given energy value is computed.

*Method of solution*
Internal and external solutions satisfying the boundary conditions in the origin and the asymptotic region, respectively, are generated by integrating the radial equation with the Fox–Goodwin method and from the mismatch of their logarithmic derivatives a correction to the eigen energy/potential strength is determined. The procedure is repeated with the corrected value till convergence. The wave function is normalized in the Zel'dovich sense by integrating numerically along a contour in the complex $r$-plane.

*Restrictions on the complexity of the problem*
The present method does not work in the vicinity of zero energy and for unphysical resonances and antibound states.

*Typical running time*
0.5–3 s per iteration.

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* Permanent address: Mathematical Institute of the Kossuth University, Debrecen, Hungary.

Computer Physics Communications 27 (1982) 385–401
North-Holland Publishing Company

# VPM – A NEW ASYMPTOTIC PACKAGE

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*Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast BT7 1NN, Northern Ireland*

Received 20 May 1982

## PROGRAM SUMMARY

*Title of program:* VPM

*Catalogue number:* AAOE

*Computer:* CRAY-1; *Installation:* SERC, Daresbury Laboratory, Warrington

*Operating system:* COS 1.10

*Programming language used:* ANSI FORTRAN 77

*High speed storage required:* 101542 words

*No. of bits in a word:* 64

*Overlay structure:* none

*Peripherals used:* card reader, lineprinter, scratch disc store, permanent disc store

*No. of cards in source program:* 3482

*Keywords:* atomic physics, asymptotic solutions, electron–atom, electron–molecule, scattering, photodetachment, free–free, variable phase, *R*-matrix, long-range potential

*Nature of the problem*
This program solves the outer region coupled equations which occur in electron–atom, electron–molecule scattering and obtains the scattering *K*-matrix together with slowing varying amplitudes from which the wavefunctions and their derivatives may readily be obtained.

*Method of solution*
The equations are solved using a method which is generally based on the variable phase method discussed by Calogero [1], but modified to take into account the peculiar features of the first order non-linear ordinary differential equations. The differential equations are solved using the powerful and stable package of Shampine and Gordon [2].

*Restrictions on the complexity of the problem*
The current version cannot treat the case of (i) a Coulombic potential, (ii) all closed channels. A modifed version to treat these cases is in preparation. Restrictions due to dimension sizes may be easily alleviated by altering PARAMETER statements (see listing for details).

*Typical running time.*
The running time depends critically upon: the number of channels included; the number of open channels; the convergence radius for the asymptotic analytic expansions employed; energies near thresholds or in resonance regions; and whether one is performing only a *K*-matrix calculation or a full *K*-matrix plus wavefunction calculation. Typically a full calculation takes approximately three times longer than a *K*-matrix only calculation. The test run took 10.5 s on the CRAY-1.

*References*

[1] F. Calogero, Variable Phase Approach to Potential Scattering (Academic Press, New York, 1967).

[2] L.F. Shampine and M.K. Gordon, Computer Solution of Ordinary Differential Equations (W.H. Freeman, San Francisco, 1974).

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Computer Physics Communications 27 (1982) 403–414
North-Holland Publishing Company

# HEVOL2: A MONTE CARLO PROGRAM TO CALCULATE THE EVOLUTION OF STRUCTURE FUNCTIONS WITH THE INCLUSION OF NEXT TO LEADING ORDER EFFECTS

A. SANSONI

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Received 6 March 1982

## PROGRAM SUMMARY

*Title of program*: HEVOL2

*Catalogue number*: AAVK

*Computer*: CDC 7600; *Installation*: CINECA, Bologna

*Operating system*: Scope 2.1.5 and NOS/BE

*Programming language used*: FORTRAN IV EXTENDED

*High speed storage required*: (40808 words) – can be varied according to the choice of parameters

*No. of bits in a word*: 60

*Overlay structure*: none

*Peripherals used*: line printer, permanent files on disk (the latter optionally, to save execution time)

*No. of cards in combined program and test deck*: 2760

*Keywords*: Monte Carlo generation, quantum chromodynamics, structure function evolution, leading logarithm approximation, next to leading logarithm approximation, heavy quark effects

*Nature of physical problem*
Calculation of the QCD evolution of structure functions including next to leading order effects with the immediate aim of determining relevant QCD parameters by least-square fits to experimental data.

*Method of solution*
Monte Carlo generation of the QCD emission of quanta by a procedure developed in ref. [1].

*Restriction on the complexity of the problem*
None in the leading log approximation. Only non-singlet analysis is implemented in the next to leading log approximation.

*Unusual features of the program*
Use of the CERN Program Library, and specifically of the minimization program MINUITS.

*Reference*

[1] R. Odorico, Phys. Lett. 102B (1981) 341.

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Computer Physics Communications 27 (1982) 415–422
North-Holland Publishing Company

# ABEL: STABLE, HIGH ACCURACY PROGRAM FOR THE INVERSION OF ABEL'S INTEGRAL EQUATION

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Received 20 May 1982

## PROGRAM SUMMARY

*Title of program*: ABEL

*Catalogue number*: AAOK

*Computer*: IBM 370/168; *Installation*: Bar-Ilan University Computer Centre, Ramat-Gan, Israel

*Operating system*: OS/MVS-3.8

*Programming language used*: FORTRAN IV G

*High speed storage required*: 45000 words

*No. of bits in a word*: 32

*Peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1614

*Keywords*: Abel equation, Abel inversion, plasma diagnostics

*Nature of the physical problem*

Abel's integral equation [1] occurs in many fields of research. In particular, in flame and plasma diagnostics it relates the emission coefficient distribution function of optically thin cylindrically symmetric extended radiation source to the line-of-sight radiance measured in the laboratory [2]. Thus, in order to obtain the physical information, which is the emission coefficient distribution function, one has to Abel-invert the measured radiance data.

*Method of solution*

Although two explicit analytic inverses are known for Abel's integral equation, their straightforward application greatly amplifies the experimental noise inherent in the radiance data [3]. This is due to the fact that these formulae employ the first derivative of the radiance function. A third, analytic inverse was recently obtained by the present authors [4] which does not require differentiation of the radiance data and thus avoids unnecessary error amplification.

Based on these three analytic inverses, three formulae were developed for computing the inverse numerically. These were obtained by representing the radiance function by a piece-wise cubic spline function [5], least squares fitted to the measured data. The inverse of Abel's integral equation for a spline function is calculated analytically, so that once the parameters of the spline are determined by the fitting procedure, the inverse can readily be calculated using either one of the three formulae. The excellent smoothing properties of the spline function insure that both error amplification [6] and over-smoothing is avoided while the piece-wise nature of the spline function keeps the termination errors small. A comparative study of our method with some of the best methods currently in use [7] indicates that for highly error-free, very noisy or sparse radiance data, our method outperforms those methods in all cases studied. The difference was, in some cases, as much as two orders of magnitude in our favour.

*Restrictions on the complexity of the problem*

Only 250 radiance values can be inverted by the present version in a single run.

*References*

[1] E.T. Whittaker and G.N. Watson, A Course in Modern Analysis (Macmillan, New York, 1948).
[2] W.L. Barr, J. Opt. Soc. Am. 52 (1962) 885.
A. Kuthy, Nucl. Instr. and Meth. 180 (1981) 7.
[3] G.N. Minerbo and M.E. Levy, SIAM J. Num. Anal. 6 (1969) 598.
[4] M. Deutsch and I. Beniaminy, Appl. Phys. Lett. 41 (1982) 27.
[5] J.H. Ahlberg, E.N. Nielson and J.L. Walsh, The Theory of

Splines and Their Application (Academic Press, New York, 1967).
[6] M.J.D. Powell, Rep. No. H267/5309 (AERE Harwell, Didcot, Oxon OX11 ORA, England, 1967).
[7] M. Deutsch and I. Beniaminy, J. Appl. Phys. (1982) (in press).

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Computer Physics Communications 28 (1982) 1–25
North-Holland Publishing Company

# FCFRKR – A PROCEDURE TO EVALUATE FRANCK–CONDON TYPE INTEGRALS FOR DIATOMIC MOLECULES

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and

U. TELLE

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Received 1 June 1982

## PROGRAM SUMMARY

*Title of program*: FCFRKR

*Computer*: SEL 32/75; *Installation*: Department of Chemistry, University of Toronto, Toronto, Canada M5S 1A1

*Operating system*: RTM 7.1

*Programming language used*: FORTRAN IV

*High speed storage required*: 64254 words (plus FORTRAN library)

*Number of bits in a word*: 32

*Peripherals used*: card reader, line printer, magnetic disc

*Number of cards in combined program and test deck*: 6958

*Keywords*: molecular, diatomic, potential curves, RKR-method, Schrödinger equation, Franck–Condon factor, Einstein $A$-value, $r$-centroid, distortion constant, dipole matrix element

*Catalogue number*: AAOR

*Nature of the physical problem*
This program package is concerned with the construction of RKR potentials and the solution of the Schrödinger equation for the nuclear motion of diatomic molecules (vibrational–rotational wave functions). The calculation of overlap integrals, Franck–Condon factors, dipole matrix elements and Einstein $A$-factors can be selected by setting the appropriate logical path switch in the program. In addition, options for the calculation of $r$-centroids and the determination of distortion constants ($D_v$ and $H_v$) are provided.

*Method of solution*
The $f$ and $g$ integrals for the evaluation of the RKR potential are obtained by numerical integration [1]. The vibrational wave functions and energy eigenvalues are evaluated from the solution of the radial Schrödinger equation for the nuclear motion of the diatomic molecule. The differential equation of second-order is transformed into a system of first-order differential equations. This allows the application of the rapidly converging correction procedure for the eigenvalues (Newton procedure) and the use of high precision integration procedures with automatic step-size control [2]. Overlap functions are calculated from tabulated eigenfunctions and operator functions (e.g. dipole moment function) applying a Simpson's integration scheme.

*Restrictions on the complexity of the problem*
Matrices for the evaluation of Franck–Condon type integrals are bounded to a field of maximum dimension of (70, 70) in order to limit the required storage area but at the same time allowing flexibility for a vast number of applications. Changes to smaller maximum dimensions or a different dimension set $(a, b)$ fitting in the reserved storage area can be easily performed. At present no options for the calculation of quasi-bound and free states are included in the procedure for the solution of the Schrödinger equation. The line-strength factors for the calculation of the Einstein $A$-factors are restricted to

singlet–singlet and doublet–doublet transitions; changes in the relevant parts of the rotational line strength formulae [3] can be acchieved without difficulties to apply the procedure to transitions of higher multiplicity.

*Typical running time*

The running time depends strongly on the requested accuracies for the evaluation of the RKR-potential and the energy eigenvalues as well as on the number of raster points in the vibrational–rotational wave function. On the average turning points for vibrational levels in the RKR-potential were computed in 0.01 (low $v$) to 0.09 (high $v$) seconds; the integration accuracy was $10^{-15}$. One iteration cycle for a wave function of 1000 raster points required $\approx 30$ s (integration accuracy $10^{-8}$). The calculation of an overlap integral between two such wave functions is usually less than 0.3 s (including time to read the wave functions from the external file).

*References*

[1] H. Telle and U. Telle, J. Mol. Spectrosc. 85 (1981) 248.
[2] R. Bulirsch and J. Stoer, Num. Math. 8 (1966) 1.
[3] I. Kovacs, Rotational Structure in Spectra of Diatomic Molecules (Adam Hilger, London, 1969).

Computer Physics Communications 28 (1982) 27–40
North-Holland Publishing Company

# ACTIV – A PROGRAM FOR AUTOMATIC PROCESSING OF GAMMA-RAY SPECTRA

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Received 14 April 1982

## PROGRAM SUMMARY

*Title of program*: ACTIV

*Catalogue number*: ABAC

*Computer*: CDC-6500 (also IBM-360, PDP-11/70); *Installation*: JINR

*Operating system*: SCOPE (CDC-6500), OS-360 (IBM), IAS (PDP)

*Programming language used*: FORTRAN IV

*High speed storage required*: 40 kwords (CDC), 200 kbytes (IMB), 32 kwords (PDP)

*Number of bits in a word*: 60 (CDC), 32 (IBM), 16 (PDP)

*Overlay structure*: required only on PDP-11/70, on others none

*No. of cards in combined program and test deck*:

*Keywords*: gamma-ray spectrum, spectrum analysis, least squares analysis, spectrum decomposition, activation analysis

*Nature of the physical problem*
Program ACTIV is intended for precise analysis of $\gamma$-ray and X-ray spectra and allows the user to carry out the full cycle of automatic processing of a series of spectra, i.e. calibration, automatic peak search, determination of peak positions and areas, identification of the radioisotopes and the transformation of the areas found into masses of isotopes in the irradiated sample. ACTIV uses a complex mathematical technique and is oriented mainly to large computers, but using overlaid loading, it can be run also on small computers like the PDP 11/70. Compared with other similar programs, ACTIV has some advantages in accuracy of peak shape description and in the reliability of the peak search and its least-square analysis. The program can be used for the purpose of activation analysis.

The program can analyze spectra with poor statistics and with broad and narrow peaks.

*Restrictions on the complexity of the program*
A multiplet should not contain more than 20 components.

*Typical running time*
1 s per single peak (CDC), 2 s (PDP).

Computer Physics Communications 28 (1982) 41–60
North-Holland Publishing Company

# A SYSTEM TO GENERATE FORTRAN PROGRAMS FOR CALCULATING CONFIGURATION TRACES OF ANGULAR MOMENTUM COUPLED PRODUCT OPERATORS *

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Received 15 March 1982

## PROGRAM SUMMARY

*Title of program*: CONTRACTION-COMPILER

*Catalogue number*: AAOP

| *Computer*: | *Installation*: |
|---|---|
| DEC VAX-11/780 | University of Toronto |
| DEC 1090 | University of Pittsburgh |
| IBM 370/3033 | Louisiana State University |

*Operating system*: VAX/VMS, TOPS-10 and MVS/SE JES2

*Programming language used*: Fortran IV

*High speed storage required*: 54 kwords

*No. of bits in a word*: 32 or 36

*Peripherals used*: magnetic disk and printer

*No. of cards in combined program and test decks: 5310*

*Keywords*: computer generated program, perturbation expansion, statistical spectroscopy, moment methods, configuration trace, operator average, normal order, Wick's expansion, correlation measure, propagation, unitary decomposition

*Nature of the physical problem*
Three steps are usually involved in setting up a problem for numerical solution,

1) deriving algebraic expressions,
2) programming the equations, and
3) debugging the codes.

Often step 1 requires repeated applications of fundamental rules, such as commutation and angular momentum recoupling in spectroscopy studies. While an individual may be able to recognize short cuts to speed up a derivation, by sheer speed and accuracy a computer programmed to manipulate the basic rules can prove to be the more effective means for deriving the algebraic expressions. Examples are given by the work reported on in refs. [1,2]. Likewise, to simplify tedious and often time-consuming task of steps 2 and 3, a code can be written to "translate" or "compile" the output of step 1 into a machine ready program. We report here on a code, called "compiler" in what follows, which accepts as input standardized output from the CONTRACTION-JT-RECOUPLING program [2] and produces, using additional information on the permutation symmetry of the operators from the CONTRACTION-

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* Work supported in part by the US National Science Foundation and Natural Sciences and Engineering Research Council, Canada.

BASIC-DIAGRAM program [1], a FORTRAN IV code for evaluating configuration traces of a product of angular momentum coupled operator.

As output from the CONTRACTION-BASIC-DIAGRAM program [1] and the CONTRACTION-JT-RECOUPLING program [2] provide input to the compiler, these two programs must be run first for each distinct operator product. This input to the compiler determines the number of basic diagrams and, for each basic diagram, the associated permutation structure, the number of summation variables, the appropriate phases and statistical weight factors, and the angular momentum recoupling information. The operators themselves are assumed to be of standard form, such as hamiltonian or electromagnetic excitation operators; all defining matrix elements are considered to be input variables. The program sets up the trace evaluation code by translating this information into Fortran IV programs. It does this by mimicking the detailed logic an individual would use if assigned the same task. Certain specific procedures that are common to many cases, such as inputing the defining matrix elements, are written as library subprograms. The compiler logic is structured but not rigid; optimization is attended to so the output codes will execute efficiently.

*Restrictions on the complexity of the problem*

The program is designed to handle up to the most complicated problems anticipated in nuclear spectroscopy studies. The basic operators must be one of the following forms:

1) $A_r$ and $B_r$, one-particle creation and annihilation operators,
2) $\Sigma_{rs} v_{rs}^{\Delta}(A_r \times A_s)^{\Delta}$ and $\Sigma_{rs} v_{rs}^{\Delta}(B_r \times B_s)^{\Delta}$, pair creation and pair annihilation operators,
3) $\Sigma_{rs} v_{rs}^{\Delta}(A_r \times B_s)^{\Delta}$, one-body (e.g., electromagnetic transition) operators, and
4) one-plus-two body interaction Hamiltonian as defined, for example, in ref. [3].

The maximum number of basic operators allowed in the product operator is 16 with no more than 8 having unitary rank [4] greater than zero and no more than two having (total) angular momentum rank greater than zero.

*References*

[1] B.D. Chang and S.S.M. Wong, Comput. Phys. Commun. 18 (1979) 35.

[2] B.D. Chang and S.S.M. Wong, Comput. Phys. Commun. 20 (1980) 191.

[3] B.D. Chang and S.S.M. Wong, Nucl. Phys. A294 (1978) 19.

[4] F.S. Chang, J.B. French and T.H. Thio, Ann. Phys. 66 (1971) 137.

Computer Physics Communications 28 (1982) 61–67
North-Holland Publishing Company

# AN EXPONENTIAL SPLINE INTERPOLATION FOR UNEQUALLY SPACED DATA POINTS

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Received 10 May 1982

## PROGRAM SUMMARY

*Title of program*: LSPLIN

*Catalogue number*: AAOW

*Computer*: HP3000 Institut für Kernphysik, HB66/80 Universität Mainz, Computer Centre

*Operating system*: HP3000 MPE IV, HB66/80 GCOS 4JS3

*Programming language used*: FORTRAN IV

*High speed storage required*: 16.8 K

*No. of bits in a word*: 16

*Peripherals used*: Nicolet-Zeta plotter

*No. of cards in combined program and test deck*: 1105

*Keywords*: interpolation, spline, *L*-spline, differentiation, quadrature

*Nature of physical problem*

Quite often it is necessary to interpolate discrete points given in an interval $[x_1, x_N]$ to some intermediate point $x \in [x_1, x_N]$ in such a way that one avoids spurious oscillations.

*Method of solution*

Instead of minimizing $\Sigma_{i=1}^{N-1} \int_{x_i}^{x_{i+1}} [f^{(2)}(x)]^2 \mathrm{d}x$, where $f$ is the interpolating function and $f^{(k)}$ is the $k$th derivative, we minimize the expression $\Sigma_{i=1}^{N-1} \int_{x_i}^{x_{i+1}} [f^{(2)}(x)]^2 + \lambda_i^2 [f^{(1)}(x)]^2 \mathrm{d}x$ with a weight parameter $\lambda_i$ which indicates the relative importance of the first derivative of the interpolating function $f$ in the minimization process.

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Computer Physics Communications 28 (1982) 69–74
North-Holland Publishing Company

# SIMULATION OF POWDER EPR SPECTRA WITH AXIAL SYMMETRY

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and

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Received 19 January 1982

## PROGRAM SUMMARY

*Title of program*: SIMULAPO

*Catalogue number*: AAOF

*Computer*: B 6800; *Installation*: Instituto Militar de Engenharia, Rio de Janeiro, Brasil

*Operating system*: WFL

*Programming language used*: FORTRAN 77

*High speed storage required*: 25000 words

*No. of bits in a word*: 52

*Overlay structure*: none

*Peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 670

*Keywords*: EPR, axial *D*-tensor, powder spectrum

*Nature of the physical problem*
The determination of the spin Hamiltonian parameters from powder spectra often requires a full simulation of the spectrum, especially when the zero-field parameters are of the same order as the Zeeman term [1]. This program calculates the first derivative of the EPR absorption spectrum of powder samples using the following approximations:

i) the paramagnetic species is randomly distributed in space;
ii) the linewidth is isotropic and is the same for all transitions.

*Method of calculation*
The single crystal spectra are calculated exactly for a large number of orientations (typically 90) of the magnetic field. These spectra are convoluted with a first-derivative line shape function and added to yield the powder spectrum.

*Restriction on the complexity of the problem*
In its present version, the program is restricted to spectra with axial symmetry ($E=0$), no hyperfine terms ($A=0$) and isotropic g. The electron spin $S$ must be in the range $1 \leq S \leq 5/2$

*Typical running time*
The running time on the B 6800 is of the order of $30S(2S+1)$ seconds, where $S$ is the electron spin. It thus ranges from 90 s (for $S=1$) to about 8 min (for $S=5/2$).

*Reference*
[1] T.I. Barry, J. Mater. Sci. 4 (1969) 485.

Computer Physics Communications 28 (1982) 75–101
North-Holland Publishing Company

# SHELL MODEL CALCULATIONS OF POINT DEFECT FORMATION ENERGIES IN CUBIC IONIC CRYSTALS

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Received 12 May 1982

## PROGRAM SUMMARY

*Title of program*: Point Defects in Cubic Ionic Crystals

*Catalogue number*: AAOL

*Computer*: Univac 1100/82

*Operating system*: EXEC 8

*Programming language used*: FORTRAN 77 double precision

*High speed store required*: up to approx. 147 Kwords

*Peripherals used*: printer

*No. of cards in program*: 4268

*Keywords*: lattice statics, point defects, cubic ionic crystals, shell model

Computer Physics Communications 28 (1982) 103–107
North-Holland Publishing Company

# ACOUSTIC PHONON ANISOTROPY: PHONON FOCUSING

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Received 29 December 1981

## PROGRAM SUMMARY

*Title of program*: ACOUSTIC PHONON ANISOTROPY

*Catalogue number*: AAOJ

*Computer*: DEC LSI 11-23

*Operating system*: RT-11 Version 3.0

*Programming language*: FORTRAN IV version 2.5

*High speed storage required*: 13 Kwords

*No. of bits in a word*: 16

*Peripheral used*: line printer

*No. of cards in program and test deck*: 1073

*Keywords*: solid state, acoustics, phonons, elastic waves, anisotropy, phonon focusing, heat-pulse

*Nature of the physical problem*
Calculation of the phase velocity, polarization vector, group velocity, and phonon-focusing enhancement factor for non-dispersive acoustic plane-waves of any wave-vector.

*Method of solution*
The group velocity and the phonon-focusing enhancement are calculated from the derivatives of the characteristic equation of the Christoffel equations.

*Restrictions on complexity*
The material must be described by a symmetric real 6-vector elastic constant matrix.

*Typical running time*
0.3 s.

*References*

[1] H.J. Maris, J. Acoust. Soc. Am. 50 (1971) 812.
[2] G.A. Northrop and J.P. Wolfe, Phys. Rev. B22 (1980) 6196.
[3] M.J.P. Musgrave, Crystal Acoustic (Holden-Day, San Francisco, 1970) p. 84.

Computer Physics Communications 28 (1982) 109–151
North-Holland Publishing Company

# LPOTT – PION AND KAON ELASTIC SCATTERING FROM SPIN $\frac{1}{2}$ NUCLEI IN MOMENTUM SPACE

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*and*
*Department of Physics, University of Surrey, Guildford, Surrey GU2 5XH, England* *

Received 1 December 1981; in revised form 9 June 1982

## PROGRAM SUMMARY

*Title:* LPOTT

*Computer:* CDC Cyber 170/72. Present version also runs on CDC 7600; *Installation:* Computer Center, Oregon State University, Corvallis, OR 97331, USA

*Operating system:* NOS 1.4

*Program language:* FORTRAN 77

*Memory required:* 132.7 $K_8$ (46.5 $K_{10}$) words to load (102 $K_8$ – LPOTT, 11 K – FORTRAN libe, rest-system), 121.7 $K_8$ (41.9 $K_{10}$) words to run

*No. of bits per word:* 60 (14–15 decimal place accuracy, 1–4 instructions/word)

*Peripherals used:* disk files (8 files on "program" card, 4 supplied with program, 1 scratch, 2 output, 1 computed and stored)

*Number of cards:* 5037 FORTRAN, 1127 input data

*Keywords:* optical potential, pion, kaon, elastic scattering, charge exchange scattering, momentum space, spin $\frac{1}{2}$ nuclei, multiple scattering theory, $\sigma(\theta)$, $\sigma^{\mathrm{tot}}$

*Method of solution*
A theoretical momentum-space optical potential is generated from elementary meson–nucleon amplitudes ** and realistic nuclear matter and spin form factors. The potential is expanded in Legendre series and the resulting one-dimensional, coupled Lippmann–Schwinger integral equations are reduced to linear equations and solved by matrix inversion. Differential and total scattering cross sections, polarizations and coordinate space wave functions are calculated for both the elastic and single charge exchange scattering of $\pi^+$, $\pi^-$, $\pi^0$, $K^+$ or $K^0$. The theory includes nuclear spin $\frac{1}{2}$ with realistic form factors, nucleon recoil and binding (2- or 3-body subenergies), Lorentz invariant relations between amplitudes and kinematic variables in different reference frames (angle and momentum transformations), the most recent elementary phase shifts, theoretical off-energy-shell behavior generated from separable potential models, Pauli effects, an "exact" inclusion of the Coulomb force, and a second-order potential to represent the effects of true absorption.

*Typical running time*
Most of the running time is used to set up the potential matrix. The test case, $\pi^+$ $^{12}$C scattering at 50 MeV with 10 partial waves, takes $\approx 20$ s without Pauli modifications and $\approx 28$ s with Pauli modifications. These times are nearly doubled for a spin $\frac{1}{2}$ nucleus, and doubled again for charge exchange since LPOTT does $\pi^+(K^+)$ and then $\pi^0(K^0)$. As the nucleus gets larger and/or the energy increases, an increase in running time approximately proportional to the increased number of partial waves will occur. However, the program saves some time by use of the Born approximation for higher partial waves.

*Restrictions*

Spin 0 $\otimes$ spin 0, spin 0 $\otimes$ spin $\frac{1}{2}$,

$0 \leq T_\pi \leq 1.5$ GeV, $0 \leq T_K \leq 1$ GeV.

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* Some subroutines written by S.C. Phatak, A.W. Thomas and M.J. Paez. Supported in part by the National Science Foundation (USA) and the Science Research Council (UK).

** Future versions of LPOTT will be published for nucleon–nucleus scattering (spin $\frac{1}{2} \otimes \frac{1}{2}$).

No. of meson–nucleus (nucleon) partial waves $\leq 30$ (8) in com. Number of grid points for numerical integration of wave equation $\leq 32$ (must modify one DIMENSION statement to increase). Exact Coulomb only for elastic scattering (not charge exchange). Variety of nuclear densities possible, but not at all energies. Variety of kinematic prescriptions possible.

Computer Physics Communications 28 (1982) 153–182
North-Holland Publishing Company

# PROGRAM PACKAGE FOR CALCULATING MATRIX ELEMENTS OF TWO-CLUSTER STRUCTURES IN NUCLEI

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Received 29 April 1982

## PROGRAM SUMMARY

*Title of program*: DFIDTH

*Catalogue number*: AAOG

*Computer*: CDC Cyber 172; *Installation*: RRC Ljubljana

*Operating system*: NOS/BE 1.3

*Programming language used*: ANSI FORTRAN (exceptions)

*High speed storage required*: 40300 words (octal) for the test version

*No. of bits in a word*: 60

*Peripherals used*: card reader, line printer, 1 permanent disk file

*No. of cards in combined program and test deck*: 269

*Keywords*: integrals over angles, partial-wave expansion, word addressable files

*Nature of physical problem*
Matrix elements of operators between Slater determinants of two-cluster structures must be expanded into partial waves for the purpose of angular momentum projection. The expansion coefficients contain integrals over the spherical angles $\vartheta$ and $\varphi$.

*Method of solution*
All integrals needed (see program PRO2C) are calculated using analytical formulae and stored in a file with the CDC Word Addressable organization. This file is used by the program PRO2C.

*Restrictions on the complexity of the problem*
No restrictions of physical nature.

*Typical running time*
1.1 s for the test run.

*Unusual features of the program*
A disk file with the CDC Word Addressable organization is used (with the Record Manager routines).

## PROGRAM SUMMARY

*Title of program*: STOKER

*Catalogue number*: AAOH

*Computer*: CDC Cyber 172; *Installation*: RRC Ljubljana

*Operating system*: NOS/BE 1.3

*Programming language used*: ANSI FORTRAN (exceptions)

*High speed storage required*: 120400 words (octal) for the test version

*No. of bits in a word*: 60

*Peripherals used*: card reader, line printer, 1 permanent disk file

*No. of cards in combined program and test deck*: 1000

*Keywords*: cluster model, symbolic algebra, symbolic-numerical information conversion, word addressable files

*Nature of physical problem*
In the cluster model, the matrix elements of operators between Slater determinants of cluster structures must be evaluated by symbolic algebra programs because of their length and number. They are the building blocks for the matrix elements between nuclear eigenfunctions of total angular momentum and parity. Therefore the symbolic expressions have to be converted to an equivalent set of numerical data and the latter stored for easy access (by program PRO2C).

*Method of solution*
A special set of subprograms reads and interprets the symbolic expressions. The numerical information so obtained is written into a file with the CDC Word Addressable organization in a space-saving form. Parts of information belonging to given operators and bra–ket clustering pairs can be accessed using pointers stored in the beginning of the file. Program STOKER can update the file many times.

*Restrictions on the complexity of the problem*
Restrictions are imposed by the symbolic expressions interpreting subprogram package. The expressions can have at most 99 terms (of the form exponential function times a polynomial in several variables) and the powers of variables in polynomials can be one-digit only. A polynomial can be at most 1000 characters long (80 characters per card). These restrictions can be removed.

*Typical running time*
1.0 s for the test run.

*Unusual features of the program*
A disk file with the CDC Word Addressable organization is used (with the Record Manager routines).

## PROGRAM SUMMARY

*Title of program*: PRO2C

*Catalogue number*: AAOI

*Program obtainable from*: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

*Computer*: CDC Cyber 172; *Installation*: RRC Ljubljana

*Operating system*: NOS/BE 1.3

*Programming language used*: ANSI FORTRAN (exceptions)

*High speed storage required*: 76 100 words (octal) for the test version

*No. of bits in a word*: 60

*Peripherals used*: card reader, line printer, 2 permanent disk files (created by programs DFIDTH and STOKER)

*No. of cards in combined program and test deck*: 2246

*Card punching code*: 29

*Keywords*: cluster model, interplay of different cluster structures, angular momentum projection, symbolic algebra, word addressable files

*Nature of physical problem*
The dynamics of a nucleus with cluster structure or with an interplay of different cluster structures lie in the corresponding Hill–Wheeler equation [1]. The kernels of this equation are matrix elements of the Hamiltonian and the identity between functions obtained from Slater determinants of cluster structures by the angular momentum and parity projection. The purpose of program PRO2C is to calculate the necessary matrix elements.

*Method of solution*
Projection of angular momentum and parity employed [1] is an algebraic one without resort to numerical integration. Matrix elements between projected functions are expressed in terms of those between unprojected ones (Slater determinants). The latter are first expanded into partial waves. Program PRO2C then uses the two files with the Word Addressable organization constructed by the programs DFIDTH and STOKER, respectively. The program is optimized with respect to time consumption.

*Restrictions on the complexity of the problem*
The present version of PRO2C allows for at most one 1p single particle state in any given cluster structure, and for at most two nucleons in the unfilled shells. These restrictions affect a comparatively small part of subprograms and can be removed (see below).

*Typical running time*
2.7 s for the test run.

*Unusual features of the program*
Two disk files with the CDC Word Addressable organization are used (with the Record Manager routines).

*Reference*

[1] M.V. Mihailović and M. Poljšak, Nucl. Phys. A311 (1978) 377.

Computer Physics Communications 28 (1982) 183–187
North-Holland Publishing Company

# COMPUTATION OF OUTER PRODUCTS OF SCHUR FUNCTIONS

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Received 17 May 1982

## PROGRAM SUMMARY

*Title of program:* Schur

*Catalogue number:* AAMJ

*Computers upon which the program is operable:* Various mini and microcomputers supporting the UCSD Pascal system

*Computer:* PDP-11/780; *Installation:* UCSD

*Operating system:* UCSD Pascal system

*Programming language used:* UCSD Pascal

*High speed storage required:* 1900 words

*Number of bits in a word:* 16

*Overlay structure:* none

*Peripherals used:* console, disk

*Number of cards in combined program and test deck:* 498

*Keywords:* Schur function, outer product, irreducible representation, partition, Ferrers' diagram, standard tableau, skew-tableau, backtracking, depth-first order, balanced tree

*Nature of physical problem*
To express the (outer) product of an arbitrary number of Schur functions as a linear combination of Schur functions.

*Method of solution*
A new backtracking algorithm [1] is implemented to generate the partitions that appear in the expansion of a product of Schur functions.

*Restrictions on the complexity of the problem*
The size of the problem that can be handled by the implementation is restricted by the total number of parts of the input partitions (no more than 255).

*Typical running time*

| | |
|---|---|
| $\{5^2\}\{3^2 2\}$ | 2 s. |
| $\{31\}\{2^2\}\{21\}\{1^2\}$ | 8 s. |

(Time indicated includes the disk-write time: 1 and 2 s, respectively.)

*Unusual features of the program*
The partitions generated by the algorithm are maintained as nodes of a balanced binary tree to minimize list insertion time.

*References*

[1] J. Remmel and R. Whitney, Multiplication of Schur Functions (to appear).
[2] D.E. Littlewood and A.R. Richardson, Phil. Trans. A 233 (1934) 99.
[3] D.E. Littlewood, The Theory of Group Characters, 2nd ed. (Oxford Univ. Press, London, 1950) p. 94.

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Computer Physics Communications 28 (1982) 189–200
North-Holland Publishing Company

# A MORE EFFICIENT VERSION OF THE WEIGHTS AND NJSYM PACKAGES

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Received 4 June 1982

## PROGRAM SUMMARY

*Title of program:* WEIGHTS – A more efficient version

*Catalogue number:* AAOM

*Computer used:* CRAY- 1; *Installation:* SERC, Daresbury Laboratory, Warrington WA4 4AD

*Operating system:* OS 1.10

*Programming language used:* ANSI FORTRAN 66

*High speed storage required:* 62571 words

*No. of bits in a word:* 64

*Peripherals used:* card reader, line printer

*No. of cards in source program:* 3047

*Reference to other published version of this program:*

| *Cat. no.* | *Reference* |
|---|---|
| ACQL | Comput. Phys. Commun. 1 (1970) 359 |
| ACQV | Comput. Phys. Commun. 2 (1971) 180 |
| ACQV | Comput. Phys. Commun. 6 (1973) 59 |
| ACQV | Comput. Phys. Commun. 7 (1974) 318 |
| ACQV | Comput. Phys. Commun. 8 (1974) 329 |

*CPC Library subprograms used:*

| *Cat. no.* | *Reference* |
|---|---|
| ACQB | Comput. Phys. Commun. 1 (1969) 15 |
| ACRN | Comput. Phys. Commun. 6 (1973) 88 |
| AAON | this paper |

*Keywords:* atomic structure, scattering, Racah coefficients, coefficients of fractional parentage, recoupling coefficient, wave functions, *LS* coupling, bound states, continuum Slater integral

*Nature of physical problem*
In configuration interaction calculations, one wishes to evaluate the matrix of the Hamiltonian operator with respect to a basis set of configuration wave functions. The more difficult part of this procedure is to determine the two-electron interaction matrix elements. These matrix elements may be written as a weighted sum of radial Slater integrals. This program calculates the coefficients of these integrals.

*Method of solution*
The coefficients of the Slater integrals are obtained from integration over all spin and angular coordinates and ($N$-2) radial coordinates, for an $N$-electron atom. The scheme for calculating the coefficients is described by Fano [1]. In this scheme, the coefficients may be expressed as sums over fractional parentage coefficients, recoupling coefficients and reduced matrix elements. A more efficient package [2] is now employed to evaluate the recoupling coefficient. This results in execution time decreasing by a factor of between three and four.

*Restrictions on the complexity of the problem*
Any number of electrons in s-, p- or d-shells are allowed ($\leqslant 2(2l+1)$), but no more than two electrons in any shell of higher orbital angular momentum. The earlier over-all restriction of $l \leqslant 4$ is lifted in this new version. The restriction on a maximum of two electrons for $l > 2$ may be relaxed by inclusion of further fractional parentage coefficient packages.

Current dimensions restrict the number of occupied subshells to a maximum of ten.

*Typical running time*
The test case took 6.6 s execution time on the CRAY-1.

*References*

[1] U. Fano, Phys. Rev. 140 (1965) A67.
[2] N.S. Scott and A. Hibbert, Comput. Phys. Commun. 28 (1982) this paper.

## PROGRAM SUMMARY

*Title of program:* NJSYM – A more efficient version

*Catalogue number:* AAON

*Computer:* CRAY-1; *Installation:* SERC, Daresbury Laboratory, Warrington WA4 4AD

*Operating system:* OS 1.10

*Programming language used:* ANSI FORTRAN 66

*High speed storage required:* 38240 words

*No. of bits in a word:* 64

*Peripherals used:* card reader, line printer

*No. of cards in the source program:* 1509

*Reference to other published version of this program:*

| *Cat. no.* | *Reference* |
|---|---|
| AAGD | Comput. Phys. Commun. 1 (1969) 241 |
| AAGD | Comput. Phys. Commun. 2 (1971) 173 |
| AAGD | Comput. Phys. Commun. 2 (1971) 181 |
| AAGD | Comput. Phys. Commun. 5 (1973) 161 |
| AAHD | Comput. Phys. Commun. 8 (1974) 151 |

*Keywords:* atomic structure, scattering, recoupling coefficients, Racah coefficient, $3n-j$ symbol, angular momentum, matrix element, angular integral

*Nature of the physical problem*
A general recoupling coefficient for an arbitary number of integer or half integer angular momenta is calculated.

*Method of solution*
The recoupling coefficient is first expressed as a sum over products of Racah coefficients multiplied by (-1) factors and $(2j+1)^{1/2}$ factors. This summation is then evaluated using an efficient Racah coefficient subroutine which is a factor of six faster than the original one employed in the NJSYM package.

*Restrictions on the complexity of the problem*
The program can be used to calculate a recoupling coefficient containing any number of angular momenta by modifying the dimensions of appropriate arrays.

*Typical running time*
The test run took 0.5 s execution time on the CRAY-1.

*Unusual features of the program*
When the program has been used once to evaluate a given recoupling coefficient it is possible to call the routine over and over again for the same coefficient with different angular momenta without re-expressing the recoupling coefficient in terms of Racah coefficients. This facility now works in all circumstances (see section 2 of the long write-up).

Computer Physics Communications 28 (1982) 201–205
North-Holland Publishing Company

# CLASSIFICATION OF AUGER-TRANSITIONS IN *LS*-COUPLING

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Received 16 June 1982

## PROGRAM SUMMARY

*Title of program*: CLASSIFICATION OF AUGER-TRANSITIONS

*Catalogue number*: AAOV

*Computer for which the program is designed and others on which it is operable*: SUPERBRAIN (INTERTEC DATA SYSTEMS), 7880 (SIEMENS)

*Operating system*: CP/M, BS3000

*Programming language used*: FORTRAN IV

*High speed storage required*: 26 kB.

*No. of bits in a byte*: 8

*Peripherals used*? terminal (interactive), printer

*No. of cards in program deck*: 1339 (including 450 cards documentation)

*Keywords*: atomic structure, *LS*-coupling, complex atoms, Auger transitions, transition probability

*Nature of physical problem*
Auger-transitions for light atoms may often be described in *LS*-coupling. This program determines whether these transitions are allowed or forbidden. In addition, information is given on the degree of forbiddenness: parity-forbidden, spin-forbidden or both. For many cases of spectrum-analysis these data together with calculated transition energies will yield sufficient information for identification of observed lines. As exact calculations of transition-probabilities for Auger-decays are often very tedious, this rough distinction between allowed and several classes of forbidden transitions may be of great help for the interpretation of experimental data.

*Method of solution*
The user defines (in an interactive session) the initial and final configurations. These are tested for physical meaningfulness. Then the possible terms for these configurations are determined following the rules of quantum-mechanical sequential angular coupling. The number of occurrences of each term is indicated. Finally, the degree of forbiddenness is determined, and the user may select all terms of a specified degree or just all degrees to be output to the selectable output-unit.

*Restrictions on the complexity of the problem*
Initial and final state are represented by a single configuration, respectively. S-, p- and d-shells with any number of electrons and f-shells with up to 3 electrons may be involved. The maximum number of orbitals is 9. The number of terms for initial or final state must not exceed 30. These limits may, however, be extended easily by enlarging the corresponding arrays on computer systems with larger storage than the SUPERBRAIN.

*Typical running time*
The typical running time on the SUPERBRAIN for test-case a) with interactive input is 100 s including loading of the program (12 s) and printing the results (40 s).

Computer Physics Communications 28 (1982) 207–215
North-Holland Publishing Company

# A PROGRAM TO SOLVE A SET OF LINEAR COUPLED DIFFERENTIAL EQUATIONS DESCRIBING A COLLISON PROCESS WITH SEVERAL ELECTRONIC AND VIBRATIONAL DEGREES OF FREEDOM

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Received 9 June 1982

## PROGRAM SUMMARY

*Title of program:* VIBREQ

*Catalogue number:* AAOX

*Installation:* SARA (Academic Computing Centre Amsterdam)

*Operating system:* NOS/BE

*Programming language:* FORTRAN IV

*High speed storage requested:* 3.5 k

*No. of bits in a word:* 60

*Peripherals used:* line printer

*No. of cards in program deck:* 1739

*Keywords:* Diabatic states, curve crossing, vibronic states, linear coupled differential equations

*Nature of physical problem*
Theoretical description of a collision process involving a number of electronic and vibrational (vibronic) states.

*Method of solution*
The coupled linear differential equations describing the system are simultaneously integrated by means of an adapted fourth-order Runge–Kutta method.

## ERRATUM NOTICE

*Titel of paper:* Simulation of EPR-spectra of randomly oriented samples
*Authors:* C. Daul, C.W. Schlapfer, B. Mohos, J. Ammeter and E. Gamp
*Reference:* Comput. Phys. Commun. 21 (1981) 385

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Computer Physics Communications 28 (1983) 229–254
North-Holland Publishing Company

# THE LUND MONTE CARLO FOR $e^+e^-$ JET PHYSICS

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Received 1 August 1982

## PROGRAM SUMMARY

*Title of program:* JETSET 4.3 E

*Catalogue Number:* AAVM

*Computer for which the program is designed and others on which it is operable:* ND, Univac, CDC and others with a FORTRAN 77 compiler

*Computer:* ND-50; *Installation:* University of Lund, Lund, Sweden

*Operating system:* SINTRAN III/VS

*Programming language used:* FORTRAN 77

*High speed storage required:* 37 Kwords

*No. of bits in word:* 32

*Peripherals used:* terminal or card reader for input, terminal or line printer for output

*No. of cards in combined program and test deck:* 1313

*CPC Library subprograms used:* JETSET 4.3 G; *catalogue number:* AAVJ

*Keywords:* $e^+e^-$ annihilation, jet fragmentation, Monte Carlo simulation, sphericity, thrust, cluster analysis

*Nature of physical problem*
In high energy $e^+e^-$ annihilation events a large number of particles are to be found in the final state. These particles are not uniformly distributed in space, but rather concentrated into a few jets. In QCD, the candidate theory of strong interactions, this is understood as the creation of a small number of quarks and gluons in the primary interaction, which then hadronize to give the jets. However, the mechanism of this hadronization is not well understood. Experimentally, it is then difficult to disentangle the perturbative aspects of QCD from the hadronization ones.

*Method of solution*
Matrix elements obtained in perturbative QCD and QFD (the standard $SU(2)\times U(1)$ theory of weak and electromagnetic interactions) are implemented to give a diescription of the production of different quark flavours, the emission of gluons and the angular orientation of partons. The program presented in a companion paper [1] is then used to take care of the jet fragmentation and particle decays. This way, we generate complete events that can be directly compared with experimental data. To help characterize these events, we also implement the ordinary sphericity and thrust measures and present a new cluster algorithm.

*Restrictions on the complexity of the problem*
Only leading order QFD and first order QCD (second order QCD if the user supplies virtual corrections) are implemented. Radiative corrections are not included, but can be added.

*Typical running time*
The matrix element treatment (i.e. the parts presented in this paper) of a continuum event at 40 GeV takes 0.015 s if four-jet events are not included and 0.03 s if they are. The subsequent jet fragmentation and particle decays (described in ref. [1]) take 0.25 s. For a toponium event at 40 GeV matrix element treatment again takes 0.015 s and the subsequent hadronization 0.35 s. Times for sphericity, thrust and cluster analysis of 40 GeV events are 0.02, 0.15 and 0.3 s, respectively. The time for four-jet treatment depends strongly on the energy, making inclusion of four-jet events quite time-consuming at higher energies, while time for hadronization and event analysis is roughly linear in multiplicity and hence slowly increasing with the energy.

*Unusual features of the program*
A random number generator is required.

*Reference*

[1] T. Sjöstrand, Comput. Phys. Commun. 27 (1982) 243.

Computer Physics Communications 28 (1983) 255–264
North-Holland Publishing Company

# CALCULATION OF DIFFERENTIAL SCATTERING CROSS-SECTIONS FOR CLASSICAL BINARY ELASTIC COLLISIONS

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Received 7 June 1982

## PROGRAM SUMMARY

*Title of program*: SCATXS

*Catalogue number*: AANX

*Computer*: DEC-2060; *Installation*: Dublin University

*Operating system*: TOPS-20

*Programming language used*: FORTRAN IV

*High speed storage required*: 9 Kwords

*No. of bits in a word*: 36, 72

*Peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 1179

*Keywords*: ion scattering spectroscopy, binary elastic collisions, differential scattering cross sections, surface physics

*Nature of physical problem*
To calculate the differential scattering cross-section and impact parameter for a classical two-body collision process involving atoms and ions, for some commonly-used interaction potentials.

*Method of solution*
Gauss–Legendre quadrature and a divided difference method.

*Restrictions on the complexity of the problem*
Repulsive potentials only may be used.

*Typical running time*
Test decks required 5 min CPU in total on a DEC-2060.

*Unusual features of the program*
Double precision arithmetic is used.

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Computer Physics Communications 28 (1983) 265–269
North-Holland Publishing Company

# EXACT PWBA VIRTUAL PHOTON SPECTRUM FOR A($\gamma_v$, D)R [+]

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Received 5 June 1982

## PROGRAM SUMMARY

*Title of program*: VPSPEC

*Catalogue number*: AAOQ

*Computer*: HP 3000; *Installation*: Institut für Kernphysik, Universität Mainz

*Operating system*: HP 3000 MPE IV

*Programming language used*: Fortran IV

*High speed storage required*: 4 K

*No. of bits in a word*: 16

*No. of cards in combined program and test deck*: 181

*Keyword*: virtual photon spectrum

*Nature of physical problem*
Quite often in nuclear and intermediate energy physics it is desirable to extract photon induced cross sections from measured electron induced cross sections. Assuming the validity of virtual photon theory this extraction can be carried out by means of a virtual photon spectrum [1,2].

*Method of solution*
The virtual photon spectrum in Plane Wave Born Approximation (PWBA) for the case of a two-body hadronic final state is an integral over electron scattering angles. For finite mass targets this integral cannot be performed analytically without making certain kinematic approximations [1,2]. Here we describe a simple computer program for the numerical integration of the virtual photon spectrum integral which makes no kinematic approximations.

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[+] Supported by the Deutsche Forschungsgemeinschaft, SFB 0201.

Computer Physics Communications 28 (1983) 271–274
North-Holland Publishing Company

# COMPUTATION OF CASIMIR OPERATOR EIGENVALUES

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Received 12 October 1981; in revised form 5 August 1982

## PROGRAM SUMMARY

*Title of program:* CASEIG

*Catalogue number:* AARX

*Computer:* CDC CYBER 173; *Installation:* Université de Montréal

*Operating system:* NOS/BE 1.4

*Programming language used:* Fortran 5

*High speed store required:* 24960 words

*No. of bits in a word:* 60

*Peripherals required:* line printer

*No. of lines in program:* 244

*Keywords:* Lie algebras, Casimir operators, irreducible representations, group symmetries, nuclear structure, elementary particles

*Nature of the physical problem*
The purpose of CASEIG is to compute the eigenvalues of Casimir operators of arbitrary order for unitary unimodular, orthogonal and sympletic groups.

*Method of solution*
CASEIG sets up an upper triangular matrix and sums the elements of $p$th power of the matrix. This sum is the eigenvalue of the Casimir operator of order $p$. Different types of classical Lie algebras differ only in the values of certain parameters appearing in the matrix. The program is based on the results of Perelomov and Popov [1].

*Restrictions on the complexity of the problem*
CASEIG uses rational arithmetic. The integers should be in the range $-[2^{48}-1]$ to $[2^{48}-1]$. The program is dimensioned for matrices of size $\leqslant 15$. This can be easily increased subject to the overflow condition.

*Typical running time*
Execution times depend on the type of Lie algebra, its rank and the irreducible representation. The compile time is 1.4 s. Test runs described in the paper require from 0.3 s to 1.9 s.

*Unusual feature of the program*
CASEIG is written in ANSI FORTRAN 77, a subset of Fortran 5 (Data statement is non-Ansi).

*Reference*

[1] A.M. Perelomov and V.S. Popov, Soviet J. Nucl. Phys. 3 (1966) 676, 819.

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Computer Physics Communications 28 (1983) 275–286
North-Holland Publishing Company

# REAL AND IMAGINARY PART OF THE HEAVY ION OPTICAL POTENTIAL FROM A REALISTIC NUCLEON–NUCLEON INTERACTION *

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Received 1 May 1982

## PROGRAM SUMMARY

*Title of program:* RIHIOP

*Catalogue number:* ABPL

*Computer:* UNIVAC 1100; *Installation:* Computing Centre, University of Tübingen

*Operating system:* EXEX LEV. 37R2A

*Programming language used:* FORTRAN

*High speed storage required:* 33 K words

*No. of bits in a word:* 32

*Pheripherals used:* card reader, line printer

*No. of cards in combined program and test deck:* 1918

*Keywords:* nuclear, heavy ion, complex optical potential, volume and surface contributions

*Nature of physical problem*
The program calculates the volume and surface contribution to both the real and imaginary parts of the optical potential between two heavy ions. The volume part is computed by a double folding procedure which uses a complex effective force as input [1–3] while the surface part is obtained as the second order term of the Feshbach expression by taking explicitly into account the excitation of a set of intermediate vibrational states [4].

*Method of solution*
Volume part: The volume part can be written as a five-dimensional integral which is calculated numerically using Gaussian quadrature.
Surface part: The surface part is written as a sum over contributions from each surface excitation state. The related Greens function is expanded in a local plane wave expansion involving a sum over partial waves. The localizing integral is calculated numerically using Gaussian quadrature.

*Restrictions on the complexity of the problem*
The number of ion–ion separation distances at which the optical potential can be computed is limited to 20. However (see input description below), any increase of this limit can easily be implemented. The projectile momentum is limited to less than 0.5 $\mathrm{fm}^{-1}$/nucleon. For the surface contributions only isoscalar vibrational states of multipolarity $\chi = 2, 3, 4$ are allowed. Isovector states of $\lambda = 1, 2, 3, 4$ can be included if the Coulomb excitation mechanism is turned on. A total of 10 excitation states only can be included (20 if the two heavy ions are identical). The heavy ions are restricted to even mass nuclei with ground state angular momentum zero.

*Typical running time*
The calculation of the grid of values of the volume potential required as input for the surface excitation subprogram takes approximately 5 min for each of the test examples. For each point required by the user an additional 40 s should be allowed for.

## References

[1] A. Faessler, T. Izumoto, S. Krewald and R. Sartor, Nucl. Phys. A359 (1981) 509.
[2] R. Sartor, A. Faessler, S.B. Khadkikar and S. Krewald, Nucl. Phys. A359 (1981) 467.
[3] R. Sartor and A. Faessler, Nucl. Phys. A376 (1982) 263.
[4] S.B. Khadkikar, L. Rikus, A. Faessler and R. Sartor, Nucl. Phys. A369 (1981) 495.

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* Supported by the Bundesministerium für Forschung und Technologie.

Computer Physics Communications 28 (1983) 287–297
North-Holland Publishing Company

# A PROGRAMMING PACKAGE FOR THE STUDY OF HIGH ANGLE GRAIN BOUNDARIES BY USING TEM

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and

P. DELAVIGNETTE

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Received 10 September 1981; in revised form 7 May 1982

## PROGRAM SUMMARY

*Titles of programs:* GB1, GB2, GB3

*Catalogue number:* AAOS

*Computer:* UNIVAC 1106; *Installation:* Computer Centre, Univ. of Thessaloniki

*Programming language used:* FORTRAN IV

*High speed storage required:* 9 K

*No. of bits in a word:* 36

*Peripherals used:* card reader, printer

*No. of cards in combined program and test deck:* 1343

*Keywords:* Polycrystalline material, grain boundaries, coincidence site lattice (CSL), transmission electron microscopy (TEM)

*Nature of the physical problem*

The study of grain boundaries by means of TEM requires first the characterization of the bicrystal, that is, the determination of the rotation relationship between the two crystals, and second the identification of the grain boundary, that is, the CSL which can be attributed to this rotation relactionship. The theoretical and the experimental methods which should follow for such a study have already been published [1–3].

*Method of solution*

The rotation operation between two grains is defined from electron diffraction patterns. The equivalent descriptions due to the symmetries are computed by matrix calculations. One of these descriptions is compared with operations leading to coincidence site lattices which are defined by integer variable analysis. The comparison between experimental and theoretical rotation operations is obtained from their matrix product taking into account the small angle criterion.

*Typical running time*

The running time (CPU time) for the test run of GB1 is approximately 14 s and for GB3 20 s for the cubic case and 14 s for the hexagonal case. The running time of GB2 depends on the number of the parameters $\alpha$ and their maximum value. In the test run the running time of the larger example is about 3 min.

*References*

[1] Th. Karakostas, G. Nouet, G.L. Bleris, S. Hagege and P. Delavignette, Phys. Stat. Sol. (a) 50 (1978) 703.
[2] Th. Karakostas, G. Nouet and P. Delavignette, Phys. Stat. Sol. (a) 52 (1979) 65.
[3] G.L. Bleris, S. Hagege, G. Nouet, J.G. Antonpoulos, Th. Karakostas and P. Delavignette, Proc. 7th Eur. Congr. on Electron Microscopy, Vol. 1, Physics (7th Eur. Congr. on El. Mc. Foundation, Leiden, The Netherlands, 1980) p. 250.

C-854

Computer Physics Communications 28 (1983) 299–314
North-Holland Publishing Company

# THE COMPUTATION OF STEADY STATE ARCS WITH MILD NOZZLE – WALL ABLATION

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Received 25 August 1982

## PROGRAM SUMMARY

*Title of program:* ARCABL

*Catalogue number:* ACEC

*Computer:* IBM 4341; *Installation:* University of Liverpool

*Operating system:* Conversational Monitor system, VM/370

*Programming language used:* Fortran IV

*High speed storage used:* 27 kwords which includes 20 kwords storage used by a NAG routine

*Number of bits in a word:* 32

*Peripherals used:* visual display unit, line printer

*Number of cards in combined test deck:* 1000

*Keywords:* electric arcs, wall ablation

*Nature of the physical problem*
The intense radiative flux from an electric arc burning in a convergent–divergent nozzle provides a mechanism by which nozzle-wall ablation may occur. The code described below finds the supercritical solution for the system shown in fig. 1. The external flow is assumed to be one dimensional and isentropic.

*Method of solution*
The three first-order ordinary differential equations describing the arc, its external flow and the ablation layer are solved using a modified form of the patching method of Fang et al. [1].

For a given set of user-specified operating conditions (e.g. current level, nozzle wall material, quenching gas, etc.) the ratio of the arc displacement area to nozzle area and that of the ablation displacement area to nozzle area (i.e. $\beta_c$ and $\beta_{ad,c}$) are guessed at the critical point. These are used to compute the position of the critical point $\zeta_c$, and the values of the Mach number at $\zeta_c$ and at the nozzle entrance. Once these are known the governing differential equations can be integrated forward from the electrode tip and backward from the critical point to a conveniently chosen patching point. The sum of the squares of the differences of the dependent variables at the patching point is then minimized with respect to $\beta_c$ and $\beta_{ad,c}$.

*Typical running time*
With reasonable guesses for $\beta_c$ and $\beta_{ad,c}$ a solution may be found within 130 s on an IBM 4341.

*Reference*

[1] M.T.C. Fang, S.K. Chan and R.D. Wright, Comput. Phys. Commun. 13 (1978) 363.

Computer Physics Communications 28 (1983) 323
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# ERRATUM NOTICE

*Title of paper*: Programs for the dynamic simulation of liquids and solids. II. MDIONS: rigid ions using the Ewald sum
*Authors*: N. Anastasiou and D. Fincham
*Reference*: Comput. Phys. Commun. 25 (1982) 159
*Title of program*: MDIONS
*Catalogue number*: AARM

*Title of paper*: Programs for the dynamic simulation of liquids and solids. II. MDIONS: rigid ions using the Ewald sum (vectorised version on the CRAY-1)
*Author*: D. Fincham
*Reference*: Comput. Phys. Commun. 25 (1982) 177
*Title of program*: MDIONS (VECTORISED)
*Catalogue number*: AARN

C-856

Computer Physics Communications 28 (1983) 337–353
North-Holland Publishing Company

# DUSTCD: A RADIATIVE TRANSPORT CODE FOR SPHERICALLY SYMMETRIC DUST CLOUDS

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Received 15 July 1982; in revised form 25 August 1982

## PROGRAM SUMMARY

*Program title:* DUSTCD

*Catalogue number:* AAEJ

*Computer:* IBM 3033; *Installation:* Rensselaer Polytechnic Institute.

*Operating system:* Michigan Terminal System.

*Programming language used:* FORTRAN

*High speed storage required:* about 50 kwords

*Number of bits in a word:* 64

*Peripherals used:* card reader, disk drive, line printer

*Number of cards in combined program and test deck: 2827*

*Keywords:* radiative transfer, interstellar matter

*Nature of physical problem*
Dust grains are an important component of the interstellar medium. Their presence in the vicinity of stars, in nebulae and in interstellar molecular clouds is confirmed by IR observations. These, coupled with accurate theoretical models, provide a key to understanding the characteristics of the thermally radiating material as well as the physics of the underlying sources which are obscured by the dust. Realistic models require the solution of the problem of photons scattered and absorbed by dust grains.

*Method of solution*
The radiative transfer problem is cast as a two-point boundary value problem. The resulting system of equations is solved by a Newton–Raphson method.

*Restrictions on the complexity of the problem*
The code will handle up to five dust components. A minimum of 60 frequency points, 55 radial points and 60 impact parameters is recommended.

*Typical running time*
For a radial grid of N points, and NF frequency points, the asymptotic estimate of running time is approximated by $N^2 * NF + N^3$). For a typical model as above, with two dust components, the computation took about 7.6 s per iteration on our IBM 3033, using FORTRAN and double precision. Hence, a typical model should require only one to two minutes of computer time. On a CDC 7600, the program should run about twice as fast.

Computer Physics Communications 28 (1983) 355–366
North-Holland Publishing Company

# A MONTE CARLO CALCULATION OF THE DISSOCIATION OF FAST $H_2^+$ IONS TRAVERSING THIN CARBON FOILS

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Received 27 July 1982

## PROGRAM SUMMARY

*Title of program:* CARLO

*Catalogue number:* AAOZ

*Computer:* IBM 4341 *Installation:* University of Toledo, Toledo, OH 43606, USA

*Operating system:* CP/CMS

*Programming language used:* OS/360 Fortran IV H Extended

*High speed storage required:* 50 Kbytes

*No. of bits in a byte:* 8

*Word length:* half word (16 bit); full word (32 bit)

*Peripherals used:* terminal, disk

*No. of cards in combined program and test deck:* 907

*Keywords:* Monte Carlo, molecular ions, molecular dissociation, Coulomb explosion, multiple scattering

*Nature of physical problem*
Calculation of the distributions of interparticle separation and relative energy for protons which result from the dissociation of fast $H_2^+$ ions traversing thin carbon foils as a function of incident ion energy and target foil thickness. Effects of Coulomb explosion in a screened Coulomb field, multiple Coulomb scattering by target atoms and differential energy loss (straggling) are included.

*Method of solution*
The problem is solved by application of Monte Carlo techniques in order to account for the simultaneous occurrence of the three processes described above.

*Restrictions*
Foils must be sufficiently thin that the total change in the energies of the incident protons is not a significant fraction of the initial value and that the final interproton separation not be so large as to be comparable with the foil thickness. With the DIMENSION statements supplied, a maximum of 500 $H_2^+$ ions can be followed through a foil in one run.

*Typical running time*
Depends upon the problem being treated. For the example provided, the number of foil slices, NS, is 545 and typical running times per event (one $H_2^+$ molecule followed through the foil) are: Coulomb explosion plus electronic straggling but no multiple scattering, 1.0 s; with multiple scattering added, 1.4 s.

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* Present address: ITT/Federal Electric Corporation, Vandenberg Air Force Base, Califonia, USA.

Computer Physics Communications 28 (1983) 367–403
North-Holland Publishing Company

# FIRE – A CODE FOR COMPUTING THE RESPONSE OF AN INERTIAL CONFINEMENT FUSION CAVITY GAS TO A TARGET EXPLOSION

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Received 8 June 1982

## PROGRAM SUMMARY

*Title of program:* FIRE

*Catalogue number:* AAHP

*Computer:* Univac 1110; *Installation:* MACC, University of Wisconsin, Madison, Wisconsin

*Operating system:* Univac 1110 EXEC VIII

*Programming language used:* FORTRAN

*High speed storage required:* 60045 words

*No. of bits in a word:* 36

*Peripherals used:* line printer, up to ten mass storage files or magnetic tapes

*No. of cards in combined program and test deck:* 3668

*Keywords:* inertial confinement fusion reactor design, gas protection concept, deposition of target X-ray, deposition of target debris, cavity gas response

*Nature of the physical problem*
One of the methods that has been suggested for protecting the first wall of a commercial inertial confinement fusion (ICF) reactor from the X-rays and ions emitted by an exploding target is to fill the cavity with a gas [1]. The FIRE code described in this article simulates the interaction of the target X-rays and ions with the gas, and computes the response of the gas to a target explosion. The results computed by the FIRE code are useful for analyzing the thermal and mechanical response of a first wall that is protected with a cavity gas.

*Method of solution*
The deposition of target X – rays into the gas is computed with an exponential attenuation model. A table of X-ray attenuation coefficients for atoms with atomic numbers ranging from 1 to 100 and X-ray energies ranging from 0.01 keV to 1 MeV is supplied with this version of the code [2]. The initial X-rays that are absorbed ionize the gas near the target, and reduce the photoelectric attenuation coefficient for subsequent X-rays. The X-ray deposition model used by the FIRE code accounts for the reduction in the attenuation coefficient with increasing ionization [3].
The internal energy and momentum transferred from the target debris to the gas are computed from the results of an ion transport code. The results of the ion transport code are fit to analytic functions, and these analytic functions are used to estimate the rates at which internal energy and momentum are deposited as functions of time and space [3].
The FIRE code simulates the response of a cavity gas to the deposition of target X-rays and ions by solving differential equations of energy and momentum conservation. These equations are solved in the Lagrangian reference frame by finite difference methods. A tabulated equation of state and tabulated Planck and Rosseland mean free paths are needed to compute the response of the gas. The MIXER code [4] has been developed to compute this data for the FIRE code. The TSTRESS code [5] then uses the heat fluxes and overpressures at the first wall computed by FIRE to analyze the response of the first wall.

*Restrictions on the complexity of the problem*
The FIRE code assumes one-dimensional symmetry in computing the interaction of the target X-rays and ions with the gas, and also in computing the gas response. The cavity gas can be divided into a maximum of 97 Lagrangian zones, and either planar, cylindrical or spherical geometry can be assumed.
The gas is assumed to be composed of only one atomic number in computing the X-ray deposition. At present, the model for computing the reduction in the photoelectric attenuation coefficient with increasing ionization is only used if the gas is neon, argon or xenon. To compute the reduction in the attenuation

coefficient for additional gases, the energy of the K, L and M shells of the neutral gas and the number of electrons in each shell must be added to the subroutine EDATA.

*Typical running time*

The CPU time required to compute the deposition of target X-rays and ions into the gas is minimal compared to the time required to compute the gas response. On the Univac 1110, the CPU time required to compute the gas response is about $2 \times 10^{-3}$ s/zone cycle.

*Unusual features of the program*

The FIRE code is written in standard FORTRAN except for the manner in which the COMMON blocks are used. The COMMON blocks are listed only at the beginning of the program, where they are equated to INCLUDE statements. Thereafter, the INCLUDE statements are used to represent the COMMON blocks. The use of INCLUDE statements abbreviates the listing of a program that uses the same COMMON blocks in many subroutines, because an INCLUDE statement occupies only one line, whereas a COMMON block might occupy many lines. INCLUDE statements only have meaning to a Univac compiler, so the user may wish to replace them with the respective COMMON blocks.

## References

[1] R.W. Conn et al., University of Wisconsin Fusion Engineering Program Report UWFDM-220 (Dec. 1977).

[2] K.G. Adams and F. Biggs, Sandia Lab., SC-RR-72-0683, Albuquerque, NM (Dec. 1973).

[3] T.J. McCarville, G.A. Moses and G.L. Kulcinski, University of Wisconsin Fusion Engineering Program Report UWFDM-406 (April 1981).

[4] R.R. Peterson and G.A. Moses, UWFDM-372, Univ. of Wisconsin (Sept. 1980).

[5] R.R. Peterson, R.D. Watson, W.G. Wolfer and G.A. Moses, UWFDM-382, Univ. of Wisconsin (Dec. 1980).

Computer Physics Communications 28 (1983) 405–426
North-Holland Publishing Company

# MIXERG – AN EQUATION OF STATE AND OPACITY COMPUTER CODE

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Received 8 June 1982

## PROGRAM SUMMARY

*Title of program:* MIXERG

*Catalogue number:* AAHO

*Computer:* Univac 1110; *Installation:* Madison Academic Computing Center, University of Wisconsin, Madison, Wisconsin, USA

*Operating system*: Univac 1110 EXEC VIII

*Programming language:* FORTRAN

*High speed storage required:* 64000 words

*No. of bits in a word:* 36

*Peripherals used:* line printer, up to ten mass storage files or magnetic tapes

*No. of cards in combined program and test deck:* 2485

*Keywords:* semiclassical atomic physics, ionization, group opacities

*Nature of the physical problem:*
The calculation of group opacities and equations-of-state of gases is important to many areas of applied physics. Specifically, to correctly predict the propagation of heat and shock waves through gases, one must have optical data, ionization states and internal energy densities for the gas [1–4]. MIXERG is a computer code which has been written to provide low cost data for mixtures of up to five gases. The optical data consists of Rosseland and Planck mean opacities or mean free paths, in single group and in multigroup form.

*Method of solution*
The ionization state of the mixture of gases is the first calculation done for each combination of plasma density and plasma temperature. This is done using the Saha model when the density is high and the temperature is low and is done using the Coronal model otherwise. Care is taken to insure that the transition between models is smooth. With the ionization state as a function of temperature, the plasma internal energy density, the heat capacity and the temperature derivative of the ionization state may be calculated. Once the state of the gas has been determined, MIXERG uses a semiclassical model to find the absorption coefficient of the plasma as a function of photon energy where photo-ionization, inverse bremsstrahlung, Thomson scattering, absorption by plasma waves and atomic line absorption are considered as absorption mechanisms. This absorption coefficient is integrated with a specially designed method to give the opacities of the plasma. The output data is stored in a manner which is easily readable by hydrodynamic codes such as FIRE [5].

*Restrictions on the complexity of the problem*
The ionization models used are only valid when the density is low enough that the electron wave functions are single atom wave functions. This means that the plasma density must be significantly less than the solid density. These models are also invalid if the plasma is not in local thermodynamic equilibrium. This sets a lower limit on the density. There are also limitations due to the absorption model. The most important inaccuracies occur at photon energies below 1 eV. This is particularly due to neglect of molecular states which may be dominant at these low energies but also comes from inaccuracies in the models used at these energies. This means that low energy group opacities and low radiation temperature single group opacities may be inaccurate.

*Typical running time*
On the UNIVAC 1110 at the Madison Academic Computer Center at the University of Wisconsin, MIXERG requires 0.4 s of CPU time for each combination of plasma density, plasma temperature and radiation temperature.

*Unusual features of the program*

The MIXERG code is written in standard FORTRAN except for the manner in which the COMMON blocks are used. The COMMON blocks are listed only at the beginning of the program, where they are equated to INCLUDE statements. Thereafter, the INCLUDE statements are used to represent the COMMON blocks. The use of INCLUDE statements abbreviates the listing of a program that uses the same COMMON blocks in many subroutines, because an INCLUDE statement occupies only one line, whereas a COMMON block might occupy many lines. INCLUDE statements only have meaning to a UNIVAC compiler, so the user may wish to replace them with the respective COMMON blocks.

*References*

[1] M.A. Sweeney and D.L. Cook, Bull. APS 24 (1979) 1072.

[2] L.A. Glenn, Lawrence Livermore Laboratory Report UCID-18573 (6 March 1980).

[3] G.A. Moses and R.R. Peterson, University of Wisconsin Fusion Engineering Program Report UWFDM-323 (October 1979): Nucl. Fusion 20 (1980) 859.

[4] R.R. Peterson, G.A. Moses and G.W. Cooper, Nucl. Tech. Fusion 1 (1981) 377.

[5] T.J. McCarville, R.R. Peterson and G.A. Moses, University of Wisconsin Fusion Engineering Program Report UWFDM-407 (June 1981, revised February 1982); Comput. Phys. Commun. 28 (1983) 367.

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North-Holland Publishing Company

# THE OLYMPUS FORTRAN COMPOSITOR

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Received 1 October 1982

## PROGRAM SUMMARY

*Title of program:* COMPOS

*Catalogue number:* ACEA

*Computer:* PRIME 750; *Installation:* Culham Laboratory. The program can be used on any computer equipped with the OLYMPUS system, and IBM support routines are provided

*Operating system:* PRIMOS

*Operating language:* ANSI Fortran 66

*High speed storage required:* 3 PRIME virtual memory segments, of 64 Kwords each (50 K used)

*No. of bits in a word: 32*

*Peripherals used:* disc

*Number of lines in combined program and test deck:* 5496

*CPC Library programs used (alternatives):*

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ABUF | OLYMPUS (ICL 4/70) | 7 (1974) 245 |
| ABUJ | OLYMPUS (IBM 370/165) | 9 (1975) 51 |
| ABUK | OLYMPUS (CDC 6500) | 10 (1975) 167 |

*Keywords:* OLYMPUS, Fortran, documentation, automatic code generation, word-processing, text formatting

*Nature of problem*
The COMPOSITOR is a word-processing program that converts a free-format Fortran input file to standardized OLYMPUS form. It is used for the semi-automatic construction and maintenance of OLYMPUS software, and can also be used for tidying-up existing Fortran codes in order to make them better structured and more readable. A variety of comment styles is allowed for.

*Method of solution*
The input file is read in A-format, line by line, and temporarily converted into unpacked integer format for processing. It is then stored in packed format prior to output.

*Restrictions on the complexity of the problem*
The COMPOSITOR is written in OLYMPUS form in ANSI Fortran 66 and should run on any type of computer system provided that the OLYMPUS system is installed and that suitable character packing and unpacking routines are available. Versions of these routines are provided for the PRIME and IBM computers. It mainly handles ANSI Fortran 66 code but could readily be extended to deal with ANSI Fortran 77 or dialect statements. It processes a sequence of subprograms one-by-one. The table sizes can be extended if required.

*Typical running time*
37.4 lines/s of CPU time on the PRIME 750, plus 0.55 s setting-up time.

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# THE OLYMPUS FORTRAN GENERATOR

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Received 18 November 1982

## PROGRAM SUMMARY

*Title of program:* GENSIS

*Catalogue number:* ACEB

*Computer:* PRIME 750; *Installation:* Culham Laboratory. The program can be used on any computer equipped with the OLYMPUS System, and IBM support routines are provided.

*Operating system:* PRIMOS

*Programming language:* ANSI Fortran 66

*High speed storage required:* 3 PRIME segments of 64 K words each (minimum size program)

*No. of bits in a word:* 32

*Peripherals used:* disc

*Number of lines in combined program and test deck:* 7759

*CPC Library programs used (alternatives):*

| *Cat. no.* | *Title* | *Ref. in CPC* |
|---|---|---|
| ABUF | OLYMPUS<br>(ICL 4/470) | 7 (1974) 245 |
| ABUJ | OLYMPUS<br>(IBM 370/165) | 9 (1975) 51 |
| ABUK | OLYMPUS<br>(CDC 6500) | 10 (1975) 167 |

*Keywords:* OLYMPUS, Fortran, documentation, automatic code generation, word-processing, text formatting

*Name of problem*
The GENSIS generator is used to construct documentation modules, COMMON blocks and other standard components of an OLYMPUS program, using as input a free-format master index file, MINDEX. This enables the OLYMPUS conventions to be maintained throughout the development phase with very little work on the part of the programmer. It can also be used in the reorganisation of existing non-OLYMPUS Fortran programs.

*Method of solution*
The MINDEX input file is read in A-format, and combined with a default file on channel NOLYMP that contains standard installation-dependent and OLYMPUS information. Strings are manipulated in both packed and unpacked form, and a system-independent ASCII collating sequence is used for the alphanumeric ordering of identifiers in indexes and COMMON blocks.

*Restrictions on the complexity of the problem*
GENSIS is written in OLYMPUS form in ANSI Fortran 66 and should run on any type of computer system provided that the OLYMPUS system is installed and that suitable character packing and unpacking routines are available. Versions of these routines are provided for the PRIME and IBM computers. The table sizes can be extended if required.

*Typical running time*

7.5 s/100 lines of input on the PRIME 750.

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# NUCADA – TWO ADAPTATIONS OF THE SYSTEM NUCORE FOR NUCLEAR STRUCTURE CALCULATIONS

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and

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Received 13 April 1982

## PROGRAM SUMMARY

*Title of program:* NUCADA

*Catalogue number:* AAOY

*Computer for which the program is designed and others on which it is operable:*

*Computer:* IBM 4341; *Installation:* Information and Computing Service, Shell, C.A.P.S.A., Buenos Aires

*Computer:* IBM 370/158-3; *Installation:* Centro de Tecnología y Ciencias de Sistemas, Buenos Aires

*Operating system:* DOS/VSE (R2.0 PUT 8005); VM/CMS

*Programming language used:* FORTRAN IV (5746-F03); FORTRAN G

*High-speed storage required:* 768000 (maximum)

*Number of bits in a word:* 32

*Peripherals used:* card reader, line printer

*Number of cards in combined program and test deck:* 2979

*CPC Library subprograms used:*

*Catalogue number:* ACWH; *Title:* MINUIT; *Ref. in CPC:* 10 (1975) 343

*Reference to other published version of this program:* Comput. Phys. Commun. 25 (1982) 237, *Catalogue number:* AARQ

*Keywords:* cluster–phonon model, cluster–core model minimization, nuclear energy levels, reduced quadrupole electric transition probabilities, reduced dipole magnetic transition probabilities, electric quadrupole moments, magnetic dipole moments, mixing ratios, branching ratios, total lifetimes

*Nature of physical problem*
Calculation of nuclear energy levels and their electromagnetic properties (transitions only between levels of the same parity). The nucleus is modelled as a cluster of a few particles and/or holes interacting with a core which in turn is either modelled as a quadrupole–octupole vibrator (cluster–phonon model) [1], or of unspecified nature (cluster–core model) [2]. The members of the cluster interact via quadrupole–quadrupole and pairing forces in the first case, and via a delta force in the second.

*Method of solution*
The Hamiltonian matrix is calculated in an appropriate basis. Then it is diagonalized with adjustable parameters determined by fitting calculated to experimental energy levels through chi-square minimization with system MINUIT [3]. The adjustable parameters are the single-particle energies and interaction strength constants in the cluster–phonon model, to which matrix elements involving the core are added in the cluster–core model. The resulting eigenvalues and eigenvectors are used to calculate electromagnetic properties of the levels.

*Restrictions on the complexity of the problem*
(1) the code for the cluster–phonon model is restricted to a maximum number of two phonons of either type. The routine which builds the configuration space is specific for the current nucleus.

(2) as in the original version of this program [4], the code depends essentially on the use of the system MINUIT [3]. Of course alternative routines may be used with the appropriate changes. Moreover, the diagonalizing routines use only non-zero matrix elements.

*References*

[1] C.A. Heras and S.M. Abecasis, Phys. Rev. C27 (1983) in press.

[2] C.A. Heras and S.M. Abecasis, Phys. Rev. submitted.

[3] F. James and M. Roos, Comput. Phys. Commun. 10 (1975) 343.

[4] C.A. Heras and S.M. Abecasis, Comput. Phys. Commun. 25 (1982) 237.

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Computer Physics Communications 29 (1983) 87–95
North-Holland Publishing Company

# TWO CENTRE OVERLAP INTEGRALS OF NUMERICAL WAVEFUNCTIONS

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and

Satya PAL
*University of Nigeria, Nsukka, Nigeria*

Received 10 March 1982

## PROGRAM SUMMARY

*Title of program*: TCOI

*Catalogue number*: ACEF

*Computer*: CDC Cyber 73; IBM 370

*Operating system*: NOS/BE; TSS

*Installation*: The University of Western Ontario; National Research Council, Canada

*Programming language used*: FORTRAN IV

*High speed storage required*: 9 kwords

*No. of bits in a word*: 60 (CDC), 32 (IBM)

*Peripherals used*: card reader, printer

*No. of cards in combined program and test deck*: 825

*Keywords*: molecular orbital, wave function, overlap integrals, ab-initio M-O

*Nature of physical problem*
The overlap integrals between the two orbitals expressed with numerical wave functions are determined using Lowdin's technique [1] as developed by Sharma [2].

*Method of solution*
A double logarithmic mesh is generated to accurately represent the wave function at either of the two centres.

*Typical running time*
The CPU time for all the test cases was ≈ 1 s. The average time per overlap integral can be considerably improved when computing several overlap integrals involving the same set of orbitals.

*References*

[1] P.-O. Lowdin, Advan. Phys. 5 (1956) 1.
[2] R.R. Sharma, J. Math. Phys. 9 (1968) 505.

Computer Physics Communications 29 (1983) 97–108
North-Holland Publishing Company

# MONTE-CARLO SIMULATION OF PURE $U(N)$ AND SU($N$) LATTICE GAUGE THEORIES WITH FUNDAMENTAL AND ADJOINT COUPLINGS *

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and

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Received 5 July 1982

## PROGRAM SUMMARY

*Title of program*: SUUNFA

*Catalogue number*: AAOT

*Computer*: CDC 6600, CDC 7600; *Installation*: University of London Computer Centre

*Operating system*: CDC NOS/BE, SCOPE

*Programming language*: FORTRAN IV with a few CDC non-standard features

*High speed storage required*: 26 K (maximum)

*Number of bits in a word*: 60

*Peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 852

*Keywords*: lattice gauge theory, $U(N)$, SU($N$), $U(N)/Z_N$ and SU($N$)$/Z_N$ gauge theories, fundamental and adjoint representations, Yang–Mills theory, Abelian- and non-Abelian gauge theories, QED and QCD models, non-perturbative effects, phase transitions, confining and deconfining phases, quark theory, statistical mechanical analogies, action per plaquette, Metropolis algorithm, Monte Carlo techniques

*Nature of the physical problem*
The program simulates thermal equilibrium for $U(N)$ and SU($N$) lattice gauge theories with couplings in both the fundamental and adjoint representations. Gauge theories on a lattice were originally proposed by Wilson [1] and Polyakov [2].

*Method of solution*
A Monte Carlo simulation of the system set up on a lattice of variable dimensionality and lattice size generates a sequence of field configurations on the lattice links. The Metropolis algorithm [3], originally developed for Monte Carlo simulations in statistical mechanics, is used to generate statistical equilibrium. New configurations are generated link by link and convergence to equilibrium is accelerated by performing the Metropolis algorithm NTMAX times on a given link before passing to the next link. The matrix for a given link is updated using a table of matrices of the correct group symmetry. The program permits the choice of a cold (ordered) or hot (disordered) start.

*Restriction on the complexity of the program*
In practice, the storage requirement is crucially connected with the array ALAT which stores the link matrices for a given configuration on the lattice. This array is placed via a LEVEL2 statement in the LARGE CORE MEMORY of the CDC 7600 computer, the statement being ignored by the CDC 6600 computer. ALAT is a complex array requiring a total storage of $2DS^DN^2$ words, where $D$ is the dimensionality of the lattice

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* The submitted manuscript was written under contract DE-AC02-76CH00016 with the US Department of Energy.

space, $S$ the number of sites per dimension and $N$ the degree of the group (i.e., $U(N)$ or $\mathrm{SU}(N)$). For efficient runs $N$ should be 2 or more. The $U(1)$ case is added to the program merely for completeness and for testing the program against other $U(1)$ programs. It is inefficient for two reasons:

(i) The heat bath method is usually more efficient than the Metropolis algorithm for $U(1)$.
(ii) The program for uniformity employs $1 \times 1$ arrays for the $U(1)$ case.

Clearly from a computer point of view the location of real or complex variables should prove more efficient than for real or complex $1 \times 1$ arrays. If a user wishes to make a series of $U(1)$ runs it would be better to use a program such as that in ref. [4] to produce the results. It should be noted that for $U(1)$ the fundamental and adjoint representations are identical. For the test run $N$, $S$, $D$ took the values 2, 4, 4, respectively. Certain other arrays in the program, to be found in COMMON BLOCKS throughout the program, and also as local arrays in subroutines MONTE and RENORM, are dependent for their dimensions on the values of $N$ and $D$. Comments in the program indicate how these arrays should be dimensioned.

*Typical running time*

The execution time increases with the number of links, the degree $N$ of the group and the number of complete Monte Carlo iterations (or "passes") through the lattice. It is also dependent on the value for NTMAX ("number of hits per link") used. It increases with NTMAX though convergence towards equilibrium is accelerated. There can be an ultimate payoff in having NTMAX fairly large, say 20. For the test run NTMAX was set 5, $S$ and $D$ set 4, and the time for the 15 SU(2) iterations shown, was 109 s (i.e. $\approx 0.1$ s per link) for the CDC 6600 computer, the CDC 7600 being approximately 5 times faster.

*References*

[1] K.G. Wilson, Phys. Rev. D10 (1974) 2455.
[2] A.M. Polyakov, Phys. Lett. 59B (1975) 82.
[3] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.
[4] R.C. Edgar, L. McCrossen and K.J.M. Moriarty, Comput. Phys. Commun. 22 (1981) 433.

Computer Physics Communications 29 (1983) 131–154
North-Holland Publishing Company

# A PROGRAM TO ANALYZE SERIES OF MÖSSBAUER SPECTRA

E. VERBIEST

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Received 24 June 1982; in revised form 6 October 1982

## PROGRAM SUMMARY

*Title of program:* MOSAUT and MOSINP

*Catalogue number:* ACEG

*Computer:* VAX11/750; *Installation:* I.K.S., Leuven University

*Operating system:* VMS

*Other computers on which it is operable:* PDP11 with RT-11 or RSX-11M operating system

*Programming language used:* FORTRAN

*High speed memory required:* 26 Kwords (PDP11)

*Number of bits in a word:* 16 (PDP11)

*Overlay structure:* yes (PDP), no (VAX)

*Peripherals used:* terminal for interactive use, storage device (preferentially a disk), optionally: line printer, plotter

*Number of cards in MOSAUT, MOSINP programs and test deck:* 5613

*Keywords:* Mössbauer spectroscopy, series of spectra

*Nature of the physical problem*
Analyze a series of Mössbauer spectra by fitting them to a function, describing the physical relations between the Lorentzians and depending on parameters of which some are freely adaptable within given limits, some adaptable within limits but required to be identical for all spectra, and some constant.

*Method of solution*
A criterion for the quality of a solution is defined (least squared chi-square of individual fits). Beginning with the starting parameter values, a sequence of spectra are chosen to be fitted and for each of those some parameters are chosen to be adaptable, to try to improve the quality of the solution. A better solution is retained. The program terminates when none of the available procedures is able to improve the quality more than some required amount.

*Restrictions on the complexity of the problem*
Maximal 10 spectra of 512 data points each. The fit function can contain 12 amplitude, 12 position and 12 line width parameters and in all 25 parameters. The maximal number of Lorentzians is 24.

*Typical running time*
Strongly dependent on the complexity of the problem varying from minutes to several hours on a PDP11/34.

*Unusual features of the program*
Files are opened by calling ASSIGN included in the FORTRAN library supplied by DEC. Two routines (PLOT1, PLOT2) call routines from a plot library and may have to be adapted to the available plotting facilities.

Computer Physics Communications 29 (1983) 155–161
North-Holland Publishing Company

# EFFICIENT IMPLEMENTATION OF THE MONTE CARLO METHOD FOR LATTICE GAUGE THEORY CALCULATIONS ON THE FLOATING POINT SYSTEMS FPS-164

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Received 6 August 1982; in final form 5 November 1982

## PROGRAM SUMMARY

*Title of program:* LATTICE

*Catalogue number:* ACEK

*Computer:* DEC VAX 11/780 and FPS-164 configuration; *Installation:* Floating Point Systems UK Ltd., Data Centre, Bracknell, Berkshire, UK

*Operating system:* DEC VAX 11/780: VMS 2.4; FPS-164: SJE–RLE C

*Programming language used:* APFTN64 – FORTRAN-77

*High speed storage required:* 124 Kwords (program + monitor)

*Number of bits in a word:* 64

*Peripherals used:* line printer

*Number of cards in combined program and test deck:* 635

*Keywords:* lattice gauge theory, Yang–Mills theory, non-Abelian gauge theory, SU(6) and SU(6)/$Z_6$ gauge theories, SU($N$) and SU($N$)/$Z_N$ gauge theories, phase transitions, statistical mechanics, Monte Carlo methods

*Nature of the physical problem*
The computer program calculates the average action per plaquette for SU(6)/$Z_6$ lattice gauge theory. By considering quantum field theory on a space–time lattice [1,2], the ultraviolet divergences of the theory are regulated through the finite lattice spacing. The continuum theory results can be obtained by a renormalization group procedure.

Making use of the FPS Mathematics Library (MATHLIB), we are able to generate an efficient code for the Monte Carlo algorithm for lattice gauge theory calculations which compares favourably with the performance of the CDC 7600.

*Method of solution*
Pure SU(6)/$Z_6$ gauge theory is simulated by Monte Carlo methods on a four dimensional space–time lattice. The system is equilibrated by the method of Metropolis et al. [3]. The FPS Mathematics Library (MATHLIB) is used to take advantage of the Floating Point Systems hardware to provide the highest speed of computation.

*Restrictions on the complexity of the program*
The only restrictions on the program are those imposed by storage limitations. The number of links in the program is given by

$$D(\text{ISIZE})^D,$$

where $D$ is the space–time dimensionality and ISIZE is the number of lattice sites in any direction. The SU($N$) matrices are complex unitary unimodular matrices with $N^2$ elements. Thus, the link matrix array has dimensions

$$N^2 D(\text{ISIZE})^D.$$

This is the largest array in the program and effectively sets the limitations on the gauge group and the size of the lattice which can be considered.

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*References*

[1] K.G. Wilson, Phys. Rev. D10 (1974) 2455.
[2] A.M. Polyakov, unpublished.
[3] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.

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Computer Physics Communications 29 (1983) 163–170
North-Holland Publishing Company

# COUNTING A SMALL NUMBER OF RADIOACTIVE ATOMS MONTE CARLO PROGRAM

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Received 23 July 1982

## PROGRAM SUMMARY

*Title of program*: Counting few radioactive atoms/3

*Catalogue number*: ABQR

*Computer*: DEC20; *Installation*: Computer Centre of the University of Turku

*Operating system*: TOPS-20

*Programming language used*: USANSI FORTRAN IV (ANSI X3.9-1966)

*High speed storage required*: 26112 words

*No. of bits in a word*: 36

*Peripherals used*: card reader and line printer

*No. of cards in combined program and test deck*: 97

*Reference to other published version of this program: Cat. no.*: AAUY; *Title*: Counting few radioactive atoms/2; *Ref. in CPC*: 17 (1979) 301

*Keywords*: nuclear physics, radioactive atoms, small samples, decays, statistical analysis, Bayesian analysis, Monte Carlo method

*Nature of physical problem*
Determination of the posterior probability $P_i$ that the rate of the production of specific radioactive atoms has been $R_i$ ($i = 1,\dots,N_R$), assuming that the number of atoms is small ($\lesssim 100$) and the *times* of the pulses from the subsequent counting of decays are known.

*Method of solution*
The Bayesian statistical analysis is used. The integration of the probabilities of multiple branches of possibilities, which are typical of the Bayesian analysis, is carried out by a fast Monte Carlo method.

*Restrictions on the complexity of the problem*
The limits are relative, depending on the available computer time.

*Typical running time*
37 s (32 s CPU).

*Unusual features of the program*
Application of a Monte Carlo method to the simulation of the production and counting of a few radioactive atoms and to the empirical Bayesian analysis.

Computer Physics Communications 29 (1983) 171–183
North-Holland Publishing Company

# ERIKA – A PROGRAM FOR THE DECOMPOSITION OF LINE SPECTRA

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Received 21 September 1982

## PROGRAM SUMMARY

*Title of program*: ERIKA

*Catalogue number*: ACEH

*Computer*: ES 1040; *Installation*: Nuclear Research Institute, Řež near Prague, Czechoslovakia

*Operating system*: OS/21.8F-MVT

*Programming language used*: FORTRAN IV

*High speed store required*: 80 kbytes

*No. of bits in a byte*: 8

*Peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 1626

*Keywords*: spectroscopy, experimental data, LSQ method, minimization, simplex method, internal conversion, Auger effect

*Nature of the physical problem*
After having measured a real line spectrum, it is necessary to decompose it into particular lines. The present program performs this task and supplies the positions and heights of all peaks.

*Method of solution*
Every line is described by an analytic function depending on several parameters (height, position and shape parameters). The optimum values of these parameters are determined by the minimization of the function $\chi^2$ using the simplex minimization method. Moreover, a background which may also be a function of several parameters is fitted, as well.

*Restriction on the complexity of the problem*
In the present version, the program is suitable for the decomposition of the internal conversion spectra. To apply it to spectra of different types, the line shape should probably be modified (see the long write-up for details). A maximum of 20 parameters can be used. The spectrum to be decomposed must be given in no more than 150 points.

*Typical runnig time*
The running time depends on the number of parameters fitted. The test run needed ≈ 8.5 min of CPU time. For more detailed information, see section 9.

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North-Holland Publishing Company

# MONTE CARLO SIMULATION OF RADIATIVE CORRECTIONS TO THE PROCESSES $e^+e^- \to \mu^+\mu^-$ AND $e^+e^- \to \bar{q}q$ IN THE $Z_0$ REGION

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and

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Received 13 September 1982

## PROGRAM SUMMARY

*Title of program*: Mustraal

*Catalogue number*: ACEJ

*Computer*: CDC; *Installation*: CYBER 173

*Operating system*: NOS/BE

*Programming language used*: ANSI FORTRAN

*High speed storage required*: 12000 words

*No. of bits in a word*: 60

*Peripherals used*: line printer

*No. of cards in combined program and test deck*: 946

*Keywords*: radiative corrections, Monte Carlo simulation, muon, quark, photon, quantum electrodynamics, electroweak theory, bremsstrahlung

*Nature of physical problem*
Radiative corrections to a process are experiment dependent. A Monte Carlo simulation of both $\mu^+\mu^-$ and $\mu^+\mu^-\gamma$ events is ideally suited for imposing any experimental cuts [1]. The MC program presented here improves on ref. [1] in two respects: it is faster and it includes $Z_0$ production in the GWS model [2].

*Method of solution*
The program decides to generate either a soft or a hard bremsstrahlung event. In both cases events are first generated according to an approximate distribution. By a weighing procedure this is transformed into the exact distribution.

*Restrictions on the complexity of the problem*
The virtual corrections take only the QED part into account. Moreover, terms of order $m_\mu/E$ (muon mass over beam energy) are neglected, which restricts the applicability at low energies. With this restriction the program can also be used for heavy charged leptons and after some changes in coupling constants for quarks.

*Typical running time*
160 events per CPU s.

*References*

[1] F.A. Berends and R. Kleiss, Nucl. Phys. B177 (1981) 237.
[2] S. Glashow, Nucl. Phys. 22 (1961) 579.
S. Weinberg, Phys. Rev. Lett. 19 (1967) 1264.
A. Salam, in: Elementary Particle Theory, ed. H. Svartholm (Almquist, Stockholm, 1968).

Computer Physics Communications 29 (1983) 201–209
North-Holland Publishing Company

# WEIGHT MULTIPLICITY FOR CARTAN CLASSES

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Received 26 July 1982

## PROGRAM SUMMARY

*Title of programs*: BCD DAM and MAIN

*Catalogue number*: ACED

*Computer*: CDC Cyber 730; *Installation*: Centro di Calcolo Interuniversitaro dell'Italia Nordorientale, Casalecchio sul Reno, Bologna, Italy

*Operating system*: NOS/BE

*Programming language used*: FORTRAN IV

*High speed storage required*: 79000 words for test run

*No. of bits in a word*: 60

*Peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 809

*Keywords*: general purpose, representation, degeneracy, Cartan classes, Lie algebra, weight

*Nature of the physical problem*

The importance of simple Lie groups in physics is well known. This program computes the multiplicity of the dominant weights in a given irreducible representation of the Cartan classes $B(N)$,$C(N)$ and $D(N)$.

*Method of solution*

Given the rank $N$ the program BCD DAM generates the program MAIN. This last program computes the multiplicity of the dominant weights in a given irreducible representation of a group $G(N)$ for the classes of Cartan $B(N)$, $C(N)$ or $D(N)$ by the reduction $G(N) \rightarrow G(N-1) \otimes U(1) \rightarrow \ldots \rightarrow G(2) \otimes (U(1))^{N-2}$.

*Typical running time*

Compile time was 12.4 s, total execution time for the test run was 6.254 s.

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Computer Physics Communications 29 (1983) 231–236
North-Holland Publishing Company

# CONCON: A CODE FOR CONSTRAINED MINIMIZATION WITHOUT DERIVATIVE COMPUTATION

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Received 15 December 1982

## PROGRAM SUMMARY

*Title of program:* CONCON

*Catalog number:* ACEM

*Computer:* CDC CYBER 835, but should work on any computer with only minor changes

*Programming language:* FORTRAN (1966)

*High speed storage required:*

CYBER 835 (60 bits per word) 5460 words
VAX 11/780 (8 bits per byte) 31180 bytes

*Peripherals used:* line printer or disk file for optional output (neither required)

*Number of cards in combined program and test deck:* 4854

*Keywords:* optimization, minimization, linear constraints, nonderivative, conjugacy

*Nature of the physical problem*
The problem is mathematical rather than physical, although the source of the mathematical problem can by any one of a number of fields of physics or engineering. The problem solved by CONCON is that of minimizing a nonlinear function $f(x)$, where $x$ may (but need not) be subject to a set of linear constraints of the form

$$c_i^{\mathrm{T}}x \geqslant b_i, \quad i=1,\ldots,m.$$

Here $x$ is a vector of $n$ variables. Some of the constraints may be equalities or they may be simple bounds $x_i \geqslant 0$, which may be written as $e_i^{\mathrm{T}}x \geqslant 0$ to fit the above form.

*Method of solution*
The method of solution is completely described in a related publication (see Buckley [2]). In the unconstrained case, the method is essentially the method of conjugate directions due to Powell [6]. This code adapts Powell's method to the case where linear constraints on the variables must be satisfied. The code also includes some of the refinements of Brent [1]. The reader is referred to ref. [2] for more details.

*Restrictions on the complexity of the problem*
There are no restrictions imposed by the code itself, except that of course the problem must fit the form stated. All work arrays which are required are passed to the subroutines; therefore, the user may make them sufficiently large to solve the problem at hand. However, it is known that there is a heuristic restriction on the method. In the unconstrained case, Powell's technique is known to suffer degradation in its performance as $n$ increases. It is hard to state a specific value for $n$ at which this occurs, since it is of course problem dependent. Nonetheless, it is probably fair to say that Powell's conjugacy method becomes significantly less effective for $n > 10$. In the constrained case, the same is likely true, although it is not $n$ that is relevant, but rather the dimension of the manifold in which the minimum occurs.

*Typical running time*
This is highly problem dependent. The only guideline here is to observe the execution time recorded when executing the test problems included with CONCON. Remember though that the evaluation of "real-live" functions may be noticeably more complex and time consuming than that of the test functions used here.

*Unusual features of the program*
The program uses a number of routines of the LINPACK package – see section 3(g).

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North-Holland Publishing Company

# MICRO/MINI COMPUTER PROGRAM FOR CALCULATING THE SQUARE ROOT OF RATIONALS AT ARBITRARY PRECISION *

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Received 18 March 1982; in revised form 15 December 1982

## PROGRAM SUMMARY

*Title of program:* RATRT, REDUSE

*Catalogue number:* ACEQ

*Computer:* DEC PDP-11/03 (and up); *Installation:* University of Windsor

*Operating system:* RT-11

*Programming language used:* PAL 11 (PDP assembler) with Fortran driver

*High speed storage required:* 32 Kbytes

*No. of bits in a word:* 16

*No. of lines in combined program and test deck:* 1802

*Keywords:* square roots, arbitrary precision, assembly language

*Nature of problem*
Calculation of square roots of arbitrary rational numbers using multiple-word number precision.

*Method of solution*
Modified Newton–Raphson and Gauss algorithms are used.

*Restrictions on complexity*
The accuracy of representation is adjustable.

*Typical running time*
Depending on the length of word block (precision specified). typically for five words 90 ms and for ten words 300 ms.

*Unusual features of the program*
The program is written as Assembly language subroutines with a Fortran driver.

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* Research supported by the Natural Sciences and Engineering Research Council of Canada.

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Computer Physics Communications 29 (1983) 245–259
North-Holland Publishing Company

# COMPLEX ZEROS OF ANALYTIC FUNCTIONS

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Received 26 May 1982

## PROGRAM SUMMARY

*Title of program*: CRTEST

*Catalogue number*: AAOO

*Computer*: CDC Cyber 170/730; *Installation*: University of Sydney. (Also Honeywell Level 66/60; *Installation*: NSW Institute of Technology, Sydney)

*Operating system*: Nos 1.4 (GCOS)

*Programming language used*: FORTRAN 77

*High speed storage required*: 14336 words (on a Cyber 170)

*No. of bits in a word*: 60 (36)

*Peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 2063

*Keywords*: general purpose, complex zero, analytic function, Cauchy's integral

*Nature of physical problem*
The subroutine CROOT in CRTEST provides a versatile means of locating the zeros (within an annular region of the complex plane) of an analytic function specified by a user-supplied subroutine. CROOT has already been successfully applied in electromagnetic diffraction theory [1], in plasma astrophysics [2] and in solar energy [3].

*Method of solution*
The method of Delves and Lyness [4] is used to evaluate recursively all zeros of the user-supplied analytic function $f(z)$ lying within a specified annulus in the complex plane. The basis of the method is to employ Cauchy's integral [5] to determine the number of zeros of $f(z)$ lying within a particular region. If this is sufficiently small, Cauchy's integral and Newton's formulae [6] are used to construct a polynomial $p(z)$ having the same zeros as $f(z)$ within the region. The zeros of the low-order polynomial $p(z)$ are evaluated by Müller's method [7], and are refined iteratively by the same method.

If $f(z)$ has a large number of zeros within the initial annulus, radial bisection is used. This continues until all zeros have been found, or until successive radii become too close. In the latter case, angular division of the annulus into sectors is commenced.

*Restrictions on the complexity of the problem*
The function $f(z)$ must be analytic within the specified annulus. The variable $z$ should be chosen so that the zeros are not too tightly clustered around a single point within the annulus. Both the function $f(z)$ and its derivative $f'(z)$ are needed, and their computer evaluation should be reasonably rapid.

*References*

[1] L.C. Botten, M.S. Craig and R.C. McPhedran, Opt. Acta 28 (1981) 1103.

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[2] R.M. Winglee, Plasma Phys. (1983) in press.

[3] L.C. Botten, R.C. McPhedran, D.R. McKenzie and R.P. Netterfield, Appl. Opt. (submitted).

[4] L.M. Delves and J.N. Lyness, Math. Comput. 21 (1967) 543.

[5] E.T. Whittaker and G.N. Watson, A Course of Modern Analysis (Cambridge Univ. Press, London, 1965) p. 119.

[6] G.A. Korn and T.M. Korn, Mathematical Handbook for Scientists and Engineers (McGraw-Hill, New York, 1968) p. 13.

[7] S.D. Conte and C. de Boor, Elementary Numerical Analysis – An Algorithmic Approach (McGraw-Hill, New York, 1980) p. 120.

Computer Physics Communications 29 (1983) 261–267
North-Holland Publishing Company

# AN EXPANSION OF COMPLICATED FUNCTIONS USING CHEBYSHEV POLYNOMIALS SUITABLE FOR FAST CALCULATION

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and

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Received 24 August 1982; in revised form 20 January 1983

## PROGRAM SUMMARY

*Title of the program:* FUNEXP

*Catalogue number:* ACEE

*Computer:* IBM 360/44; *Installation:* Centro Atómico Bariloche Computer Center

*Operating system:* IBM 44PS

*Programming language:* FORTRAN IV

*High speed storage required:* 1 Kwords

*No. of bits in a word:* 32

*No. of cards in combined program and test deck:* 692

*Keywords:* fast evaluation, Chebyshev polynomials, recurrence relations, function expansion

*Nature of the physical problem*
When solving physical and mathematical problems on a computer, one or more complicated functions many have to be evaluated a great number of times. For the sake of computational efficiency it is then desirable to have a fast and compact algorithm for the evaluation of such functions.

*Method of solution*
Low-order power expansions of high accuracy are used. These are obtained via known relations from Fourier–Chebyshev series in a set of ad hoc chosen intervals. The program described in this paper performs the following tasks.

1) It partitions user-specified argument ranges (macro-intervals) in a given number of small subintervals.
2) In these subintervals, it evaluates the coefficients of Chebyshev expansions up to sixth order.
3) It rearranges the Chebyshev expansions into power series expansions, and computes, per subinterval, the average and maximum error in a given number of points.

*Restrictions on the complexity of the program*
The only restrictions on the programs are the number of subintervals in each macrointerval (NI). The combination number, given by 2*NI+132, must not exceed the dimension of the working vector. In the present version, the working vector has been dimensioned to 1000. However, this can readily be changed by the user.

*Typical running time*
The full test run took 34 s on the IBM 360/44.

[*] Fellowship granted by CNEA.
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Computer Physics Communications 29 (1983) 269–285
North-Holland Publishing Company

# PROGRAMS ‘CELESTE’ AND ‘STELLA’ FOR COMPUTATIONS IN SPECIAL RELATIVITY: EVALUATION OF THE CELESTIAL VIEW FROM AN INTERSTELLAR SPACECRAFT

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Received 29 April 1982; in final form 20 January 1983

## PROGRAM SUMMARY

*Title of programs*: CELESTE (batch-processing version); STELLA (time-sharing terminal version)

*Catalogue number*: AACI

*Computer*: CDC Cyber 71/Cyber 170-720; *Installation*: University of Lowell Computer Center

*Operating system*: FORTRAN-IV EXTENDED (ANSI 1966)

*Programming language used*: FORTRAN-IV

*High speed storage required*: 22 Kwords

*No. of bits in a word*: 60

*Peripherals used*: terminal (LA36 DECwriter II) for STELLA; card reader (model 405), line printer (model 512) for CELESTE; optional colour display console for direct display of astroscapes

*No. of lines in combined program and test deck*: program CELESTE has 462 lines, STELLA has 470 lines; star data file NEARDAT has 92 lines, CONDAT has 35 lines, YALSTAR has 520 lines, STARDAT has 2289 lines

*Keywords*: astroscape, starscape, star plot, celestial view, special relativity, length contraction, time dilation, aberration, parallax, Doppler effect, Doppler shift, brightness, apparent magnitude, stellar temperature, spectral type, colour bolometric correction, spaceflight, interstellar travel, astronavigation

*Nature of physical problem*
CELESTE and STELLA have been compiled to evaluate the celestial fore and aft views from a spacecraft in relativistic motion, aimed in any specified direction and located at any given distance from the solar system (i.e., Earth). The calculations take account of the special-relativistic effects of space contraction, aberration, parallax, Doppler shift of wavelength (colour) [including shift of infra-red stellar sources into the visible region], and perceived brightness (i.e., apparent visual magnitude). The output may, at option, provide a printed astroscape diagram as well as a tabulation of numerical results. The output data may be fed to a colour display console for a direct visual display.

*Method of solution*
Using special-relativistic formulae [1,2], the programs convert input data for stars, e.g., visible and infra-red sources (stellar coordinates, distances, spectroscopic class, apparent visual and infra-red magnitudes) into a polar representation of the fore and aft view as a function of craft speed and direction and distance [3,4].

*Restrictions on the complexity of the problem*
While the programs have been designed to deal with infra-red as well as visible stellar sources, including appropriate bolometric corrections to determine the apparent visual magnitude (perceived brightness), they do not contain similar procedures for ultra-violet sources (since at present only piecemeal data on these are available). The input file for stellar data has been restricted to stars of 4th magnitude or brighter, in order to keep the length of the star catalogue to below 5 500 entries. It could, however, be expanded at will. The programs do not provide side views, but could readily be modified to furnish these if desired.

*Typical running time*
Less than 1 min in batch mode; 2–3 min in interactive-terminal mode when no plots are generated, 5 min in terminal mode with plots.

[1] R.W. Stimets and E. Sheldon, J. Brit. Interplanetary Soc. - Interstellar Studies 34 (1981) 83.
[2] E. Sheldon and R.W. Stimets, Nukleonika (in press).
[3] R.A. Schorn, Sky and Telescope 62 (1981) 530.
[4] E. Sheldon and R.H. Giles, J. Brit. Interplanetary Soc. - Interstellar Studies 36 (1983) 99.

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Computer Physics Communications 29 (1983) 287–299
North-Holland Publishing Company

# SEURAT: A MONTE-CARLO ALGORITHM FOR CALCULATING NEUTRAL GAS TRANSPORT IN NON-CIRCULAR AXISYMMETRIC TOROIDAL PLASMAS

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Received 30 September 1982

## PROGRAM SUMMARY

*Title of program*: SEURAT

*Catalogue number*: ABSI

*Computer*: CRAY-1; *Installation*: Magnetic Fusion Energy Computer Center (MFECC), Lawrence Livermore Laboratory, Livermore, CA

*Operating system*: CRAY Timesharing System (CTSS)

*Programming language used*: FORTRAN (ANSI 66)

*High speed storage required*: 72 112 words

*No. of bits in a word*: 64

*Peripherals used*: line printer

*No. of cards in combined programs and test decks*: 3625

*Keywords*: plasma physics, thermonuclear fusion, tokamak, two-dimensional, Monte Carlo, neutral gas

*Nature of physical problem*
Calculation of mass and energy transport by neutral particles in toroidally symmetric plasmas with non-circular poloidal cross sections.

*Method of solution*
Monte Carlo simulation of neutral particle flights through a fixed plasma, with scoring by a pseudo-collisional algorithm.

*Restrictions on the complexity of the problem*
SEURAT has been applied to a wide variety of tokamak simulations, and contains a variety of checks which terminate the computation if it goes outside the range of validity of the model. A number of common input errors are checked for at the beginning of each computation.

*Typical running time*
A typical case, CPC2 described in section 7, required 4.451 CPU s on the CTSS.

*Unusual features of the program*
SEURAT is a subroutine package designed for easy incorporation into general transport codes. It is written in 1966 ANSI standard FORTRAN [1]. The machine word length is assumed to be ⩾ 32 bits throughout, except for a pseudo-random number generator included for test comparisons, which assumes word length ⩾ 36 bits. SEURAT uses a binary file generated by the auxiliary code SIGMAV described in section 2. OLYMPUS variable name spelling conventions are used [2], but no other OLYMPUS conventions or utilities are utilized. A driver is included for stand-alone operation.

*References*

[1] ANSI FORTRAN X3.9-1966, American National Standards Institute (1966).
[2] J.P. Christiansen and K.V. Roberts, Comput. Phys. Commun. 7 (1974) 245.

Computer Physics Communications 29 (1983) 301–306
North-Holland Publishing Company

# A GENERAL PROGRAM TO COMPUTE TWO ELECTRON REPULSION INTEGRALS

Peter HABITZ and Enrico CLEMENTI

*IBM Corporation, Department D55/Building 996-2, Poughkeepsie, NY 12602, USA*

Received 30 September 1982

## PROGRAM SUMMARY

*Title of program*: PP-I-1982

*Catalogue number*: ACEL

*Computer*: IBM 370/3033

*Operating system*: VM or MVS

*Programming language*: Fortran IV. A small assembler package can be substituted, with some cost of flexibility. High speed storage required: 1.5 Mbytes for effective use. Larger storage, will increase performance, smaller requires small program changes

*No. of bits in a word*: 64/32; the program is written in double precision arithmetic

*Peripherals used*: line printer, magnetic disk

*No. of cards in combined programs and test deck*: 6000

*Key words*: molecular, integrals, Cartesian Gaussian basis, ab initio computations

*Nature of physical problem*
Ab initio computations (Hartree–Fock and configuration interaction) of the electronic structure of molecules need evaluation of the two electron repulsion integrals. PP-I-1982 (Poughkeepsie Program-Integrals-1982) calculates these with Cartesian Gaussian basis functions.

*Method of solution*
All contribution to the final integral which are only dependent of the product of two basis functions are stored on two large files. The final integral computation is only a merging of those two files.

*Typical running time*
The running time is strongly dependent on the special problem as discussed in the long write-up.

*Restrictions on the complexity of the problem*
The program is designed to handle Cartesian Gaussian functions up to f-functions, and up to 100 atomic centres.

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Computer Physics Communications 29 (1983) 307–319
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# ATOMDIAT – A PROGRAM FOR CALCULATING VARIATIONALLY EXACT RO-VIBRATIONAL LEVELS OF "FLOPPY" TRIATOMICS

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Received 20 September 1982; in revised form 15 November 1982

## PROGRAM SUMMARY

*Title of program:* ATOMDIAT

*Catalogue numbers:* ACEN

*Computer:* IBM 4341/2: *Installation:* Universitair Rekencentrum Nijmegen

*Operating systems:* MVS release 3.7

*Programming language used:* FORTRAN IV

*High speed storage required:* case dependent

*No. of bits in a byte:* 8

*Overlay structure:* yes

*Peripherals used:* card reader, line printer, up to 4 optional disk files

*No. of cards in program and test desk:* 3706

*Keywords:* ro-vibrational, body-fixed, associated Laguerre polynomials, associated Legendre polynomials, Gauss–Laguerre quadrature, orthogonalised Lanczos, LC-RAMP, variational, close-coupled equations

*Nature of physical problem*
ATOMDIAT calculates the bound ro-vibrational levels of a triatomic system using body-fixed coordinates. The embedded coordinates are appropriate to atom–diatom systems and the diatom bondlength may be frozen [1].

*Method of solution*
A basis set is constructed as the product of Morse oscillator functions (associated Laguerre polynomials) for the radial coordinate(s) and associated Legendre polynomials for the bending coordinate, with rotation matrices representing the rotations. The method is variational and the parameters used in constructing the radial basis set(s) can be optimized [1,2]. A secular matrix is constructed by use of Gauss–Laguerre integration for the radial coordinate(s) and analytic integration for the angular coordinates. This matrix is diagonalised to give the solutions. A choice of Givens–Householder and orthogonalised Lanczos procedures are supplied with the program [2].

*Restrictions on the complexity of the problem*
The size of matrix that can practically be diagonalised. The program allocates arrays dynamically at execution time and in the present version the total space available is a single parameter which can be set as required.

*Typical running time*
Running times are case dependent but dominated by the time required for diagonalising the secular matrix. A problem with 350 basis functions (which can be held in 512 K) takes 7 min on the IBM 4341/2.

*Unusual features of the program*
A user supplied subroutine containing the potential energy as an (analytic) Legendre polynomial expansion is a program requirement.

*References*

[1] J. Tennyson and B.T. Sutcliffe, J. Chem. Phys. 77 (1982) 4061.
[2] J. Tennyson and B.T. Sutcliffe, J. Chem. Phys. (1983) in press.

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* Present address: SERC Daresbury Laboratory, Daresbury, Warrington, Cheshire WA4 4AD, UK.

Computer Physics Communications 29 (1983) 333–339
North-Holland Publishing Company

# A PROGRAM FOR THE CALCULATION OF LANDAU–ZENER CROSS SECTIONS AND RATE COEFFICIENTS

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Received 5 January 1983

## PROGRAM SUMMARY

*Title of program:* LZRATE

*Catalogue number:* AACJ

*Computer 1:* VAX 11/780; *Installation:* Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, USA

*Computer 2:* IBM 3033: *Installation:* Argonne National Laboratory, Argonne, Illinois, USA

*Operating systems:* VMS and MVS, respectively

*Programming language used:* FORTRAN IV

*High speed storage required:* approximately 40 Kbytes

*No. of bits in a byte:* 8

*Peripherals used:* video or hard-copy terminal and disk store, or card reader and line printer

*No. of cards in source program:* 651

*Keywords*: charge exchange, charge transfer, cross sections, exponential integrals, ionic-covalent interactions, ionic recombination, Landau–Zener, mutual neutralization, scattering

*Nature of the problem*

The Landau–Zener (LZ) approximation is a widely used procedure for estimating the cross sections and rate coefficients for a number of collision processes which are describable in terms of potential curve crossings. Among them are charge transfer [1] and mutual neutralization [2,3]. The LZ method has the advantage of requiring only a minimum of information about the physical system under consideration; furthermore calculations are very inexpensive.

*Method of solution*

The main equations in refs. [1–3] have been programmed. Accurate and efficient procedures have been implemented for the calculation of exponential integrals, and of Maxwellian averages of the same. Much of the information required was available in the numerical analysis literature but had not been applied to this problem. The present computer code will calculate LZ cross sections or rates in a few milliseconds of processor time and should run on almost any computer which has a FORTRAN compiler. It was written for atomic physicists or astrophysicists wishing to calculate cross sections or rates at the planning stage of an experiment, or to carry out a survey of a particular class of atomic processes in order to identify which of those would warrant calculation by more elaborate techniques.

*Restrictions on the complexity of the problem*

No more than 20 cross sections or rate coefficients can be calculated by the current version in a single run.

*Typical running time*

About 5 ms per cross section on the VAX 11/780 (0.4 ms on the IBM 3033). About twelve times as long for a rate coefficient.

*References*

[1] D.R. Bates and T.J.M. Boyd, Proc. Phys. Soc. London A69 (1956) 910.
[2] D.R. Bates and B.L. Moiseiwitsch, Proc. Phys. Soc. London A67 (1955) 805.
[3] S.E. Butler and A. Dalgarno, Astrophys. J. 241 (1980) 838.

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Computer Physics Communications 29 (1983) 341–350
North-Holland Publishing Company

# A PASCAL PROGRAM FOR CALCULATING THE REDUCED COULOMB GREEN'S FUNCTIONS AND THEIR PARTIAL WAVES

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Received 1 January 1983

## PROGRAM SUMMARY

*Title of program:* RCGF

*Catalogue number:* ACEP

*Computer:* CDC 6000; *Installation:* Computer Centre CYFRONET, Institute of Nuclear Research, Otwock, Świerk 05-400, Poland

*Operating system:* SCOPE 3.4.4

*Programming language used:* PASCAL 6000

*High speed storage required:* $54000_8$ words

*No. of bits in a word:* 60

*Peripheral used:* card reader, lineprinter

*No. of cards in combined program and test deck:* 1385

*Keywords:* reduced Coulomb Green's function, perturbation theory, hydrogen-like atoms

*Nature of physical problem*
The reduced Coulomb Green's function is the coordinate space representation of the sum over intermediate states encountered in bound state second order perturbation theory. This function does not depend on the particular perturbation problem. Thus, it is useful to have it calculated once. When the perturbation Hamiltonian is decomposed into terms of definite angular momentum it is useful to have the partial waves of the Green's function. We therefore present a program for calculating the functions in question.

*Method of solution*
The formulae for the reduced Coulomb Green's function and its partial waves are lengthy and tedious to evaluate [1,2]. However, these functions can be expressed in terms of polynomials multiplied by known transcendental functions: exponentials, an exponential integral and a logarithm. The main task of the program is to evaluate the coefficients of the polynomials. It is worth stressing that the results are purely analytical and exact because of the use of special data structures, for example a fraction represented by a pair of integers or a polynomial by an array of fractions.

*Restrictions on the complexity of the problem*
The value of the main quantum number $n$ ranges from 1 to 7, and that of the angular momentum quantum number $l$ from 0 to 7. These restrictions are caused by the limitations of integer arithmetic implemented in the computer used.

*Typical running time*
Compilation – 11 s, evaluation of the reduced function – 1.6 s, evaluation of the partial wave – 0.8 s.

*References*

[1] A. Lusakowski and M. Suffczynski, Bull. Acad. Pol. Phys. Astron. 28(2) (1980).
[2] M. Suffczynski, A. Lusakowski and J. Mlodzki, Bull. Acad. Pol. Phys. Astron. 28(2) (1980).

Computer Physics Communications 29 (1983) 351–359
North-Holland Publishing Company

# MOLECULAR ASSOCIATIONS

Serafin FRAGA

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Received 20 January 1983

## PROGRAM SUMMARY

*Title of program:* AMYR

*Catalogue number:* ACEO

*Computer for which the program is designed and others on which it is operable:* Amdahl 580/5860 and IBM-type computers; also FPS-190L

*Computer:* Amdahl 580/5860; *Installation:* University of Alberta Computing Services

*Operating system:* MTS

*Programming language used:* Fortran IV

*High speed storage required:* 104 Kwords

*No. of bits in a word:* 32

*Peripherals used:* disks, printer

*No. of lines in combined program and test deck:* 2198

*Keywords:* molecular interactions, $1/R$ expansion, steepest-descent energy minimization

*Nature of the physical problem*
Determination of the stable conformations of the association of two molecules.

*Method of solution*
The stable conformation(s) of the molecular association is (are) found by minimization of the energy of interaction between the two molecules. The energy is evaluated by means of a $1/R$ expansion (with $R^{-1}$, $R^{-4}$, $R^{-6}$ and $R^{-12}$ terms), with coefficients obtained by fitting of accurate SCF results [1]. The energy minimization is carried out by a steepest-descent method.

*Restrictions on the complexity of the problem*
Calculations should be restricted to molecules consisting of atoms belonging to the thirty classes for which expansion coefficients are available.

*Typical running time*
310 s for the test run (with three cases).

*Unusual features of the program*
This program has been prepared from a version, in operation at the University of Alberta, which runs on a FPS-190L array processor and produces the plots of the conformation of the molecular complex on a Tektronix T-4015-1 terminal adapted with a hard copier. The original program may be easily regenerated from this published version.

*Reference*

[1] S. Fraga, J. Comput. Chem. 3 (1982) 329.

Computer Physics Communications 29 (1983) 361–374
North-Holland Publishing Company

# CHPACK: A PACKAGE FOR THE MANIPULATION OF CHEBYSHEV APPROXIMATIONS

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*International School for Advanced Studies, Trieste, Italy*

Received 10 February 1983

## PROGRAM SUMMARY

*Title of program*: CHPACK

*Catalogue number*: ACER

*Computer*: CDC CYBER 170/720; CDC CYBER series; *Installation*: University of Trieste Computing Centre

*Operating system*: NOS 2.0

*Programming language used*: FORTRAN V

*High speed storage required*: 44 Kwords for the test program

*No. of bits in a word*: 60

*No. of lines in combined program and test deck*: 2240

*Keywords*: general purpose, minimax approximation, approximation, Chebyshev polynomials, Chebyshev series, integration, linear differential equations

*Nature of physical problem*
In several physical problems a function is required at many points. If its computation is time consuming it can better to replace it with a suitable approximation.

*Method of solution*
The present package uses the technique of Chebyshev series development to evaluate an approximation to a function of one variable on an arbitrary interval. It allows evaluation of the coefficients of the series with assigned accuracy, and manipulations of the series (sum and product of two series, integration, derivation). A routine of the package solves a linear differential equation provided that the coefficients of the equation can be expanded in Chebyshev series. An error estimate is provided in all cases.

*Restriction on the complexity of the problem*
The only restriction is the maximum number of coefficients that can be evaluated, which has been fixed at 124 (this number plays a role only in routine CHCOEF, and can be easily changed as it appears only in a PARAMETER statement), and the maximum relative accuracy (1.E–13), which is connected with the word length.

*Typical running time*
The evaluation of 128 coefficients of a cosine took 0.1 s, including the time for 128 cosine calls. The solution of differential equations depends heavily on the order of the equations and the number of coefficients involved (in general between 1 and 6 s, see the test runs). The product of two Chebyshev series of 70 terms took 0.13 s; the remaining routines execute in less than 0.01 s.

Computer Physics Communications 29 (1983) 375–390
North-Holland Publishing Company

# NUDENS: A NILSSON–BARDEEN–COOPER–SCHRIEFFER CODE AT FINITE NUCLEAR TEMPERATURE

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Received 24 January 1983

## PROGRAM SUMMARY

*Title of program*: NUDENS

*Catalogue number*: ABQS

*Computer*: IBM 370/168 and Olivetti-Hitachi OH-5480; *Installation*: ENEA, Via G. Mazzini 2, Bologna, Italy

*Operating system*: MVS/SP1 (the code does not depend on the operating system)

*Programming language used*: FORTRAN IV

*High-speed storage required*: 94 Kbytes (25 500 words)

*No. of bits in a word*: 32

*Peripherals used*: card reader, line printer, two permanent files on disk (units 20 and 21, both card-image)

*No. of line in combined program and test deck*: 1804

*Keywords*: grand canonical formalism, nuclear shell model, pairing interaction, nuclear temperature, entropy, level densities

*Nature of physical problem*
Microscopic formalism (NBCS approximation) for the calculation of nuclear thermodynamic functions, especially level densities versus excitation energy and angular momentum. A blocking effect due to unpaired nucleons in odd-$A$, or odd–odd nuclei is explicitly worked out [1,2].

*Method of solution*
A system of nonlinear equations is solved at zero and finite nuclear temperature in order to determine pairing correlation functions and chemical potentials, to be introduced in grand canonical traces, from which thermodynamic functions are derived. Excitation energy, total angular momentum and ground state correlation functions are taken as input parameters.

*Restrictions on the complexity of the problem*
Neutron–proton pairing correlations are neglected: therefore, the formalism should be applied to medium and heavy nuclei ($A \geq 50$). Collective enhancements of nuclear level densities are introduced in a simplified phenomenological form. The equilibrium shape of the nucleus is not allowed to change with excitation energy.

*Typical running time*
The execution time is strongly problem dependent. The test run requires 1 min 20 s on OH-5480 and 1 min 38 s on IBM 370/168: in this case nuclear level densities are computed at three different excitation energies.

*Unusual features of the program*
NUDENS uses the mathematical subroutine NS01AD from the Harwell Subroutine Library [3], in order to solve a system of $n$ nonlinear equations in $n$ unknowns. This subroutine is included in the deck.

*References*

[1] G. Maino, E. Menapace and A. Ventura, Nuovo Cimento 57A (1980) 427.
[2] V. Benzi, G. Maino and E. Menapace, Nuovo Cimento 66A (1981) 1.
[3] Harwell Subroutine Library, Catalogue Compiled by M.J. Hopper, Report AERE-R 7477 (1973).

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Computer Physics Communications 29 (1983) 391–415
North-Holland Publishing Company

# DWBA CALCULATIONS OF CONTINUUM SPECTRA OF NUCLEAR REACTIONS

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*Department of Physics *, University of Texas, Austin, TX 78712, USA*

Received 5 November 1982; in revised form 17 February 1983

## PROGRAM SUMMARY

*Title of program*: ORION-TRISTAR-1

*Catalogue number*: ABNL

*Computer*: CDC Dual Cyber System; *Installation*: University of Texas Computation Center

*Operating system*: UT2D

*Programming language used*: FORTRAN IV

*High speed store required*: 20224 words

*Number of bits per word*: 60

*Overlay structure*: yes

*Number of magnetic tapes required*: 3

*Other peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 3445

*Keywords*: nuclear, light ion, direct nuclear reactions to continuum region, transfer reaction, inelastic scattering, cross section, analyzing power, form factor, spectroscopic density, zero-range DWBA

*Nature of physical problem*
ORION-TRISTAR-1 calculates the angle dependent continuum cross sections, for reactions induced by light ions. For the case of a polarized spin 1/2 projectile, it also calculates the analyzing power of the continuum. It can calculate further the cross sections for leaving the residual nucleus at varying excitation energies, as well as with a range of spin $I$ and its projection $M$. These cross sections may be used as inputs for extended versions of Hauser–Feshbach type calculations. ORION produces DWBA (Distorted Wave Born Approximation) cross sections for a range of transferred angular momenta. They are multiplied in TRISTAR with corresponding spectroscopic densities, and are then added together, to obtain continuum cross sections.

*Restrictions on the complexity of the problem*
The program may rather safely be used for light ions, whose incident energies do not exceed 30–40 MeV, if the reaction is of the inelastic or pickup type. For stripping type reactions, the breakup cross section might have to be added, in order to fit experimental spectra at the higher energy end and at smaller angles. For all three types of reactions, a Hauser–Feshbach cross section would have to be added to fit data at the lower energy end of the spectrum.

*Typical running time*
The running time is roughly proportional to the maximum value of the transferred angular momentum, and also to the number of different $Q$-values, for which ORION calculates DWBA cross sections. The CPU time for the first example given in the present paper was about 14 s. A CDC DUAL CYBER 170/750 was used.

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* Work supported in part by the US Department of Energy.

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## ERRATUM NOTICE

*Title of paper* : Calculation of photoemission spectra for surfaces of solids
*Authors* : J.F.L. Hopkinson, J.B. Pendry and D.J. Titterington
*Reference* : Comput. Phys. Commun. 19 (1980) 69
*Title of program* : PEOVER1
*Catalogue number* : ACZY

Computer Physics Communications 30 (1983) 31–36
North-Holland Publishing Company

# ILUCG2: SUBPROGRAMS FOR THE SOLUTION OF A LINEAR ASYMMETRIC MATRIX EQUATION ARISING FROM A 9-POINT DISCRETIZATION

A.I. SHESTAKOV and D.V. ANDERSON

*National Magnetic Fusion Energy Computer Center (NMFECC), Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*

Received 18 April 1983

## PROGRAM SUMMARY

*Title of program*: ILUCG2 (Incomplete *LU* factorized Conjugate Gradient algorithm for 2D problems)

*Catalogue number*: ACEU

*Computer*: Cray-1; *Installation*: NMFECC, Livermore

*Programming language used*: FORTRAN

*Operating system*: CTSS

*High speed store required*: at least 22 * mn where mn is the number of linear equations

*Number of bits in a word*: 64

*Peripheral used*: printer

*Number of card images in combined program and test file*: 1193 (599 and 594 in the general source and standard FORTRAN source, respectively)

*Keywords*: partial differential equations, elliptic, parabolic, two-dimensional, plasma physics, implicit, preconditioned, conjugate gradient algorithm, ICCG, ILUCG, asymmetric matrix, non-symmetric matrix

*Nature of the physical problem*
Elliptic and parabolic partial differential equations which arise in plasma physics applications (as well as in others) are solved in two dimensions. Plasma diffusion, equilibria and phase space transport (Fokker–Planck equation) have been treated by these methods [1–3]. These problems share the common feature of being stiff and requiring implicit solution techniques. Generally, the resulting matrix equations are asymmetric; we solve them here with the ILUCG2 program. In a subsequent article we describe a simpler and faster algorithm, ICCG2, which should be used when the matrix is symmetric [4].

*Method of soltion*
A generalization of the incomplete Cholesky conjugate gradient (ICCG) algorithm is used to solve the linear asymmetric matrix equation [5,6].

*Restrictions on the complexity of the problem*
The discretization of the two-dimensional PDE and its boundary conditions must result in a spatial 9-point operator stencil which can be represented by a block tridiagonal matrix composed of tridiagonal blocks.

*Typical running times*
These are problem dependent because ill-conditioned matrices will require more iterations than well conditioned ones. However, the running times per iteration are known. For enough equations (1189 here) the time for the incomplete *LU* factorization is 5.9 μs per unknown. Each conjugate gradient iteration requires 4.2 μs per unknown. In the three test problems the number of iterations required to reach a relative residual error of $10^{-10}$ (in the L2 norm) ranged from 9 to 208.

*Unusual features of the program*
The loops are arranged to vectorize on the Cray-1 (with the CFT compiler) wherever possible. Recursive loops (which cannot be vectorized) are written for optimum scalar speed. Some of these loops were made more efficient by increasing the arithmetic per pass and at the same time reducing the number of passes. This trick significantly reduced loop overhead and made these scalar loops 30% faster.

*References*

[1] R.W. Harvey, M.G. McCoy, J.Y. Hsu and A.A. Mirin, Phys. Rev. Lett. 47 (1981) 102.

C-892

[2] D.V. Anderson and D.C. Barnes, J. Comput. Phys. 42 (1981) 288.
[3] B.G. Logan, A.A. Mirin and M.E. Rensink, Nucl. Fusion 20 (1980) 1613.
[4] D.V. Anderson and A.I. Shestakov, Comput. Phys. Commun. 30 (1983) 37.
[5] J.A. Meijerink and H.A. van der Vorst, Math. Comput. 31 (1977) 148.
[6] D.S. Kershaw, J. Comput. Phys. 26 (1978) 43.

Computer Physics Communications 30 (1983) 37–42
North-Holland Publishing Company

# ICCG2: SUBPROGRAMS FOR THE SOLUTION OF A LINEAR SYMMETRIC MATRIX EQUATION ARISING FROM A 9-POINT DISCRETIZATION

D.V. ANDERSON and A.I. SHESTAKOV

*National Magnetic Fusion Energy Computer Center (NMFECC), Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*

Received 18 April 1983

## PROGRAM SUMMARY

*Title of program*: ICCG2 (Incomplete Cholesky factorized Conjugate Gradient algorithm for 2D symmetric problems)

*Catalogue number*: ACEV

*Computer*: Cray-1; *Installation*: NMFECC, Livermore

*Programming language used*: FORTRAN

*Operating system*: CTSS

*High speed store required*: at least 14 * mn where mn is the number of linear equations

*Number of bits in a word*: 64

*Peripheral used*: printer

*Number of card images in combined program and test file*: 1012 (510 and 502 in the general source and standard FORTRAN source, respectively)

*Keywords*: partial differential equations, elliptic, parabolic, two-dimensional, plasma physics, implicit, preconditioned, conjugate gradient algorithm, ICCG, symmetric matrix, incomplete Cholesky method

*Nature of the physical problem*
Elliptic and parabolic partial differential equations which arise in plasma physics applications (as well as in others) are solved in two dimensions. Plasma diffusion, equilibria and phase space transport (Fokker–Planck equation) have been treated by these methods [1–3]. These problems share the common feature of being stiff and requiring implicit solution techniques. Sometimes, the resulting matrix equations are symmetric; we solve them here with the ICCG2 coding. In a previous article we described a slower more general algorithm, ILUCG2, which must be used when the matrix is asymmetric [4].

*Method of solution*
The incomplete Cholesky conjugate gradient (ICCG) algorithm is used to solve the linear symmetric matrix equation [5,6].

*Restrictions on the complexity of the problem*
The discretization of the two-dimensional PDE and its boundary conditions must result in a spatial 9-point operator stencil which can be represented by a symmetric block tridiagonal supermatrix composed of elementary tridiagonal matrices.

*Typical running times*
These are problem dependent because ill-conditioned matrices will require more iterations than well-conditioned ones. However, the running times per iteration are known. For enough equations (1189 here) the time for the incomplete Cholesky factorization is 4.8 μs per unknown. Each conjugate gradient iteration requires 2.4 μs per unknown. In the three test problems the number of iterations required to reach a relative residual error of $10^{-10}$ (in the L2 norm) ranged from 8 to 75.

*Unusual features of the program*
The loops are arranged to vectorize on the Cray-1 (with the CFT compiler) wherever possible. Recursive loops (which cannot be vectorized) are written for optimum scalar speed. Some of these loops were made more efficient by increasing the arithmetic per pass and at the same time reducing the number of passes. This trick significantly reduced loop overhead and made these scalar loops 30% faster.

*References*

[1] R.W. Harvey, M.G. McCoy, J.Y. Hsu and A.A. Mirin, Phys. Rev. Lett. 47 (1981) 102.

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[2] D.V. Anderson and D.C. Barnes, J. Comput. Phys. 42 (1981) 288.
[3] B.G. Logan, A.A. Mirin and M.E. Rensink, Nucl. Fusion 20 (1980) 1613.
[4] A.I. Shestakov and D.V. Anderson, Comput. Phys. Commun. 30 (1983) 31.
[5] J.A. Meijerink and H.A. van der Vorst, Math. Comput. 31 (1977) 148.
[6] D.S. Kershaw, J. Comput. Phys. 26 (1978) 43.

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North-Holland Publishing Company

# ILUCG3: SUBPROGRAMS FOR THE SOLUTION OF A LINEAR ASYMMETRIC MATRIX EQUATION ARISING FROM A 7, 15, 19 OR 27 POINT 3D DISCRETIZATION

D.V. ANDERSON

*National Magnetic Fusion Energy Computer Center (NMFECC), Lawrence Livermore National Laboratory, Livermore, CA 94550, USA*

Received 18 April 1983

## PROGRAM SUMMARY

*Title of program*: ILUCG3 (Incomplete *LU* factorized Conjugate Gradient algorithm for 3D asymmetric problems)

*Catalogue number*: ACEW

*Computer*: Cray-1; *Installation*: NMFECC, Livermore

*Programming language used*: FORTRAN

*Operating system*: CTSS

*High speed store required*: At least 15 * MN to 59 * MN (depending on the version) where MN is the number of linear equations

*Number of bits in a word*: 64

*Peripheral used*: printer

*Number of card images in combined program and test file:* 1857 (1206 are in the general source and 651 in the standard FORTRAN example)

*Keywords*: partial differential equations, elliptic, parabolic, three-dimensional, plasma physics, implicit, preconditioned, conjugate gradient algorithm, ICCG, ILUCG, asymmetric matrix, non-symmetric matrix

*Nature of the physical problem*
Elliptic and parabolic partial differential equations which arise in plasma physics applications (as well as in others) are solved in three dimensions. Plasma diffusion, equilibria and phase space transport (Fokker–Planck equation) [1–3] have been treated by similar methods in two dimensions using the codes ICCG2 [4] and ILUCG2 [5]. These problems share the common feature of being stiff and requiring implicit solution techniques. Generally, the resulting matrix equations are asymmetric; we solve them here with the ILUCG3 program. In a subsequent article we describe a simpler and faster algorithm, ICCG3, which should be used when the matrix is symmetric [6].

*Method of solution*
A generalization of the incomplete Cholesky conjugate gradient (ICCG) algorithm is used to solve the linear asymmetric matrix equation [7,8].

*Restrictions on the complexity of the problem*
The discretization of the three-dimensional PDE and its boundary conditions must result in a spatial operator with a 7, 15, 19 or 27 point stencil which can be represented by a block tridiagonal supermatrix composed of block-tridiagonal submatrices whose elements are elementary tridiagonal matrices. The resulting sparse matrix has 7, 15, 19 or 27 non-zero diagonals.

*Typical running times*
These are problem dependent because ill-conditioned matrices will require more iterations than well conditioned ones. However, the running times per iteration are known. For enough equations (1287 here) the running times per iteration per equation become independent of the number of equations. Also, the running times depend on which of the 16 versions we are using. In the test problems, which we regard as typical, the time for the incomplete *LU* factorization ranged from 4.4 to 34.0 μs per unknown for the versions that employed 7-banded and 27-banded *LU* sparsity patterns, respectively. Each conjugate gradient iteration required from 3.5 to 21.2 μs per unknown; these times depend strongly on the sparsity pattern of *LU* and weakly on that of *M*. In the test problems the number of iterations required to reach a relative residual error of $10^{-10}$ (in the L2 norm) ranged from 8 to 34.

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*Unusual features of the program*
The loops are arranged to vectorize on the Cray-1 (with the CFT compiler) wherever possible. Recursive loops (which cannot be vectorized) are written for optimum scalar speed. Some of these loops were made more efficient by increasing the arithmetic per pass and at the same time reducing the number of passes. This trick significantly reduced loop overhead and made these scalar looops 30% faster. One of the sources is not in standard FORTRAN; we show how to make it standard.

*References*

[1] R.W. Harvey, M.G. McCoy, J.Y. Hsu and A.A. Mirin, Phys. Rev. Lett. 47 (1981) 102.
[2] D.V. Anderson and D.C. Barnes, J. Comput. Phys. 42 (1981) 288.
[3] B.G. Logan, A.A. Mirin and M.E. Rensink, Nucl. Fusion 20 (1980) 1613.
[4] D.V. Anderson and A.I. Shestakov, Comput. Phys. Commun. 30 (1983) 37.
[5] A.I. Shestakov and D.V. Anderson, Comput. Phys. Commun. 30 (1983) 31.
[6] D.V. Anderson, Comput. Phys. Commun. 30 (1983) 51.
[7] J.A. Meijerink and H.A. van der Vorst, Math. Comput. 31 (1977) 148.
[8] D.S. Kershaw, J. Comput. Phys. 26 (1978) 43.

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# ICCG3: SUBPROGRAMS FOR THE SOLUTION OF A LINEAR SYMMETRIC MATRIX EQUATION ARISING FROM A 7, 15, 19 OR 27 POINT 3D DISCRETIZATION

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Received 18 April 1983

## PROGRAM SUMMARY

*Title of program*: ICCG3 (Incomplete Cholesky factorized Conjugate Gradient algorithm for 3D symmetric problems)

*Catalogue number*: ACEX

*Computer*: Cray-1; *Installation*: NMFECC, Livermore

*Programming language used*: FORTRAN

*Operating system*: CTSS

*High speed store required*: at least 13 * MN to 33 * MN (depending on the version) where MN is the number of linear equations

*Number of bits in a word*: 64

*Peripherals used*: printer

*Number of card images in combined program and test file*: 1582 (1008 are in the general source and 574 in the standard FORTRAN example)

*Keywords*: partial differential equations, elliptic, parabolic, three-dimensional, plasma physics, implicit, preconditioned, conjugate gradient algorithm, ICCG, ILUCG, symmetric matrix, incomplete Cholesky method

*Nature of the physical problem*
Elliptic and parabolic partial differential equations which arise in plasma physics applications (as well as in others) are solved in three dimensions. Plasma diffusion, equilibria and phase space transport (Fokker–Planck equation) [1–3] have been treated by similar methods in two dimensions using the codes ICCG2 [4] and ILUCG2 [5]. These problems share the common feature of being stiff and requiring implicit solution techniques. Sometimes, the resulting matrix equations are symmetric; we solve them here with the ICCG3 program. In a previous article we described a slower and more general algorithm, ILUCG3, which must be used when the matrix is asymmetric [6].

*Method of solution*
A generalization of the incomplete Cholesky conjugate gradient (ICCG) algorithm is used to solve the linear symmetric matrix equation [7,8].

*Restrictions on the complexity of the problem*
The discretization of the three-dimensional PDE and its boundary conditions must result in a spatial operator with a 7, 15, 19 or 27 point stencil which can be represented by a symmetric block tridiagonal supermatrix composed of block-tridiagonal submatrices whose elements are elementary tridiagonal matrices. The resulting sparse symmetric matrix has 7, 15, 19 or 27 non-zero diagonals.

*Typical running times*
These are problem dependent because ill-conditioned matrices will require more iterations than well-conditioned ones. However, the running times per iteration are known. For enough equations (1287 here) the running times per iteration per equation become independent of the number of equations. Also, the running times depend on which of the 16 versions we are using. In the test problems, which we regard as typical, the time for the incomplete Cholesky factorization ranged from 3.8 to 25.9 μs per unknown for the versions that employed 7-banded and 27-banded $L$ sparsity patterns, respectively. Each conjugate gradient iteration required from 1.9 to 10.9 μs per unknown; these times depend strongly on the sparsity pattern of $L$ and weakly on that of $M$. In the test problems the number of iterations required to reach a relative residual error of $10^{-10}$ (in the L2 norm) ranged from 8 to 18.

*Unusual features of the program*
The loops are arranged to vectorize on the Cray-1 (with the CFT compiler) wherever possible. Recursive loops (which cannot be vectorized) are written for optimum scalar speed. Some of these loops were made more efficient by increasing the arithmetic per pass and at the same time reducing the number of passes. This trick significantly reduced loop overhead and made these scalar loops 30% faster. One of the sources is not in standard FORTRAN; we show how to make it standard.

*References*

[1] R.W. Harvey, M.G. McCoy, J.Y. Hsu and A.A. Mirin, Phys. Rev. Lett. 47 (1981) 102.
[2] D.V. Anderson and D.C. Barnes, J. Comput. Phys. 42 (1981) 288.
[3] B.G. Logan, A.A. Mirin and M.E. Rensink, Nucl. Fusion 20 (1980) 1613.
[4] D.V. Anderson and A.I. Shestakov, Comput. Phys. Commun. 30 (1983) 37.
[5] A.I. Shestakov and D.V. Anderson, Comput. Phys. Commun. 30 (1983) 31.
[6] D.V. Anderson, Comput. Phys. Commun. 30 (1983) 43.
[7] J.A. Meijerink and H.A. van der Vorst, Math. Comput. 31 (1977) 148.
[8] D.S. Kershaw, J. Comput. Phys. 26 (1978) 43.

Computer Physics Communications 30 (1983) 59–69
North-Holland Publishing Company

# A PROGRAM FOR CALCULATION OF THE E1, E2 AND M1 TRANSITION PROBABILITIES IN ODD–ODD NUCLEI TAKING THE CORIOLIS MIXING INTO ACCOUNT

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and

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*Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, USSR*

Received 1 November 1982

## PROGRAM SUMMARY

*Title of program:* CORIOP

*Catalogue number:* ABQT

*Computer:* CDC 6500; *Installation:* Laboratory of Calculating Techniques and Automation, Joint Institute for Nuclear Research, Dubna, USSR

*Operating system:* NOS/BE 1

*Programming language used:* FORTRAN

*High speed storage required:* 125024 B words

*No. of bits in a word:* 60

*Peripherals used:* card reader, line printer

*No. of cards in combined program and test deck:* 1980

*CPC library subprogram used:*

*Catalogue number:* ACWH; *Title:* MINUIT; *ref. in CPC:* 10 (1975) 343

*Keywords:* nuclear, Coriolis effect, fitting, experimental, energy level, deformed nuclei, odd–odd nuclei, gamma transition

*Nature of physical problem*

It is well known that comparison of experimental reduced transition probabilities with their model-dependent predictions is of great importance for studying nuclear structure. Namely, the influence of the Coriolis particle-rotational coupling on electromagnetic transitions between excited states in odd-*A* deformed nuclei has been the subject of interest in many papers and has been reliably demonstrated [1]. The analogous situation in odd–odd nuclei has also been established [1].

The program makes it possible to calculate the E1, E2 and M1 reduced transition probabilities in odd–odd deformed nuclei. The mixed wave functions used result from a least-squares fit of energy levels (taking the Coriolis effect into account) to the experimental ones, performed with the modified ODDODDCORI subprogram [2].

*Method of solution*

The calculation of the reduced electromagnetic probabilities can be subdivided into two stages. In the first stage, the total Hamiltonian (with Coriolis coupling term included) is diagonalised and eigenvalues and eigenvectors are found. This procedure is described in ref. [2]. In the second, the coupling amplitudes obtained in the first stage are used for the calculation of the electromagnetic operator matrix elements, performed with the present program.

*Restriction on the complexity of the problem*

The current version is dimensioned for 40 transitions. For further restrictions see ref. [2].

*References*

[1] A. Bohr and B.R. Mottelson, Nuclear Structure II (Benjamin, New York, 1974).
[2] Z. Hons and J. Kvasil, Comput. Phys. Commun. 24 (1981) 161.

Computer Physics Communications 30 (1983) 71–85
North-Holland Publishing Company

# PHOCHA: A MONTE CARLO PROGRAM TO CALCULATE THE CHARACTERISTICS OF A BEAM OF PHOTONS PRODUCED BY ANNIHILATION AND BREMSSTRAHLUNG OF RELATIVISTIC POSITRONS

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and

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Received 20 December 1982

## PROGRAM SUMMARY

*Title of program*: PHOCHA

*Catalogue number*: AAVN

*Computer*: CDC 7600; *Installation*: CINECA Bologna. The program has also been run on the computer DEC VAX-11/780, with a word length of 32 bits

*Operating system*: CDC Scope 2.1.5 and NOS/BE

*Programming language used*: FORTRAN IV EXTENDED

*High speed storage required*: 3000 Kwords

*No. of bits in a word*: 60

*Peripherals used*: mass storage, line printer

*No. of cards in combined program and test deck*: 1481

*Keywords*: intermediate energy photon beam; in flight positron annihilation and bremsstrahlung; Monte Carlo calculation

*Nature of the physical problem*
The program PHOCHA calculates the absolute energy spectra, the radial and vertical profiles and the angular distributions of annihilation and bremsstrahlung photons from intermediate energy positrons. The energy spread, the energy loss and the multiple scattering of the positrons in the annihilation target are taken into account. Moreover the positron emittance, the positron incidence angle and the finite angular acceptance of the photon collimation channel are explicitly considered.

*Method of solution*
A positron, whose energy is extracted according to a given energy distribution, impinges on the target, flying in a given direction. The radiation point is determined according to the positron beam emittance and by a uniform extraction in the effective target thickness. Positron multiple scattering and energy loss are then sampled according to the appropriate laws. In order to minimize photon losses, the photon emission angle is extracted, for each positron, within a variable solid angle whose size and orientation are calculated by taking into account the positron flight direction and the photon production point in the target; moreover a number of photons proportional to the selected solid angle is always sampled.

*Typical running time*
In the test program set-up (positron energy 200 MeV, positron beam incidence angle on the target 0°, no. of collimators 8, about 25 photon histories for each of the 5000 sampled positrons) 271 s of CDC-7600 CPU time are required to reach a statistical accuracy better than 2% on the photon spectra.

*Unusual features of the program*
Use of the CERN program library: subroutines: MXMPY, POLROT, VMATR; functions: RNDM.

*Restrictions on the complexity of the problem*
a) the equations of the radial and the vertical phase-space ellipses of the positron beam are used in the canonical form;
b) the incoming and outcoming target surfaces are assumed to be plane;
c) bremsstrahlung straggling is not considered.

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# PROGRAM TO CALCULATE ELASTIC GREEN'S FUNCTIONS, DISPLACEMENT FIELDS AND INTERACTION ENERGIES IN CUBIC MATERIALS

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Received 20 December 1982

## Program summary

*Title of program*: CFCUBE

*Catalogue number*: ACMS

*Computer*: IBM

*Operating system*: MVS

*Programming language used*: FORTRAN IV

*High speed storage required*: 56 kbytes

*Peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 353

*Keywords*: solid state, elasticity, point defect, Green's function displacement field, interaction energy

*Nature of physical problem*

In linear elasticity theory a continuous medium is characterized by its Green's function. In the static case this Green's function can be calculated by a one-dimensional integration. Also calculated are the first two derivatives yielding displacement fields and interaction energies of point defects.

*Method of solution*

The three-dimensional Fourier integral defining the Green's function is reduced to a one-dimensional integral [1].

*Restriction on the complexity of the problem*

The method is valid for all cubic materials independent of the magnitude of the anisotropy.

*Typical running time*

0.04 s per distance for Green's function and displacements, 0.6 s per distance for interaction energy.

*Reference*

[1] D.M. Barnett, Phys. Stat. Sol. (b) 49 (1972) 741.

Computer Physics Communications 30 (1983) 93–99
North-Holland Publishing Company

# LSFBTR: A SUBROUTINE FOR CALCULATING SPHERICAL BESSEL TRANSFORMS

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Received 1 November 1982; in revised form 11 February 1983

## PROGRAM SUMMARY

*Title of program*: LSFBTR

*Catalogue number*: AANZ

*Computer*: Cyber 170-835; *Installation*: The University of Western Ontario Computing Centre

*Operating system*: NOS 2

*Programming language used*: USANSI FORTRAN IV

*High speed storage required*: 979 words for subroutine; 11442 words for test program

*No. of bits in a word*: 60

*Peripheral used*: line printer for test run

*No. of cards in combined program and test deck*: 370

*Keywords*: Hankel transforms, spherical Bessel functions, momentum space wave functions

*Nature of physical problem*
Transforming an angular momentum wave function from coordinate to momentum representation requires the calculation of Hankel transforms for spherical Bessel functions. This subroutine calculates such integrals when the function to be transformed is given numerically at $r$ values that are distributed uniformly in the variable $\ln(r)$. The resulting values of the transform are given at $k$ values distributed uniformly in the variable $\ln(k)$.

*Method of solution*
The transform can be carried out as two successive Fourier transforms that are calculated numerically using the trapezoidal rule. For meshes with a large number of points these can be calculated very efficiently using the fast Fourier transform method.

*Restrictions on the complexity of the problem*
The method is most effective for functions which have only a few nodes and have continuous derivatives on $(0, \infty)$. For other functions a very large number of mesh points may be required.

*Typical running time*
The program required 0.146 s to calculate the transform at 256 mesh points in the $l = 0$ case on the CYBER 170-835. In the $l = 5$ case the same calculation required 0.172 s. The first time the program is called for a particular mesh, about 0.3 s is required for initialization.

*Unusual features of the program*
Remarkably accurate results are obtained for very large values of the transform variable.

*Reference*

[1] J.D. Talman, J. Comput. Phys. 29 (1978) 35.

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Computer Physics Communications 30 (1983) 101–105
North-Holland Publishing Company

# SPECTROSCOPIC ENERGY COEFFICIENTS FOR VIBRATION–ROTATIONAL STATES OF DINUCLEAR MOLECULES

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Received 24 May 1982; in revised form 10 March 1983

## PROGRAM SUMMARY

*Title of program*: YDY84C

*Catalogue number*: ACET

*Computer for which the program is designed and others on which it is operable*: any computer having a FORTRAN-77 compiler and sufficient core (overlaying may be necessary but is easily effected)

*Computer*: Univac 1100/82; *Installation*: Computer Services Centre, Australian National University, Canberra, A.C.T. 2601, Australia

*Operating system*: EXEC-8 or OS1100

*Programming language used*: FORTRAN-77 with double precision

*High speed storage required*: none (16000 words was available on Univac 1100/82)

*No. of bits per word*: 36

*Overlay structure*: optional

*Peripherals used*: card reader or input terminal, line printer

*No. of cards in combined program and test deck*: 5408

*Keywords*: molecular, dinuclear, potential-energy function, spectroscopic energy coefficients

*Nature of physical problem*
The spectroscopic energy coefficients $Y_{kl}$ and their derivatives with respect to the parameters are calculated from a known set of the parameters: coefficients $c_j$ $(1 \leqslant j \leqslant 10)$ in the potential-energy function [1], and harmonic vibrational, $\omega_e$, and rotational, $B_e$, quantities.

*Method of solution*
Explicit expressions for the contributions to $Y_{kl}$ and their derivatives are used in a list scanned once in order to generate the specified quantities.

*Restrictions on the complexity of the problem*
The length of the program is compensated by separation of the intensive calculations into ten subroutines that can be overlaid or executed in segments. Depending on the parameters supplied, the generated values may lie within the range $10^{6}-10^{-80}$.

*Typical running time*
0.9 s.

*Reference*
[1] J.F. Ogilvie, Proc. Roy. Soc. (London) A378 (1981) 287.

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* Present address: Bahrain University College, Department of Chemistry, P.O. Box 1082, Manama, Bahrain.

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## ERRATUM NOTICE

*Title of paper*: VMOMS – a computer code for finding moment solutions to the Grad–Shafranov equation
*Authors*: L.L. Lao, R.M. Wieland, W.A. Houlberg and S.P. Hirshman
*Reference*: Comput. Phys. Commun. 27 (1982) 129
*Title of program*: VMOMS
*Catalogue number*: ABSH

Computer Physics Communications 30 (1983) 151–161
North-Holland Publishing Company

# EXLAM, A PROGRAM FOR THE CALCULATION AND EXPANSION OF LOCAL MODEL EXCHANGE POTENTIALS

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Received 13 January 1982; in revised form 18 October 1982

## PROGRAM SUMMARY

*Title of program:* EXLAM

*Catalogue number:* AANY

*Computer*: IBM 370/158; *Installation:* University of Oklahoma

*Operating system:* OS/V52 Release 3.8

*Programming language used:* Fortran IV

*High speed storage required:* 82000 words

*Number of bits in a word:* 32

*Peripherals used:* card reader, disk, line printer

*Number of cards in combined program and test deck:* 4300

*CPC Library Programs used:*

*Catl. no.:* ACZW and ACZX; *ref. in CPC:* 21 (1980) 63 and 79

*Keywords:* electron–molecule scattering, molecule, local model exchange potential, Legendre expension, charge density

*Nature of the physical problem*
The free-electron-gas and semiclassical local model exchange potentials [1] are calculated. The resulting model exchange potential is expanded in Legendre polynomials in a single-center coordinate system.

*Method of solution*
The model exchange potentials are determined by evaluating their analytic forms [1] at the desired set of points. The expansion in Legendre polynomials is carried out using a 32-point Gauss–Legendre quadrature [2].

*Restrictions on the complexity of the problem*
Only systems with axially symmetric charge densities are allowed.

*Typical running time*
Less than 30 s of CPU time was required to calculate either model exchange potential for the ground state of $H_2$ on a 200 point $r$-mesh. Three Legendre polynomials were used in the expansion of the exchange potential. The static potential expansion coefficients were added to those of the model exchange potential to create a total potential.

*References*

[1] T.L. Gibson and M.A. Morrison, J. Phys. B 14 (1981) 727.
[2] M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions (National Bureau of Standards, Washington, 1964).

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Computer Physics Communications 30 (1983) 163–167
North-Holland Publishing Company

# NON-ADIABATIC TRANSFORMATION OF QUANTUM-CHEMISTRY ENERGY HYPERSURFACES

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Received 7 February 1983

## PROGRAM SUMMARY

*Title of the program*: DIAB

*Catalogue number*: ABXA

| *Computer*: | *Installation*: |
|---|---|
| IBM 370/168-3033 | Universita di Pisa, Italy<br>CIRCE, Orsay, France |
| MODCOMP Classic/78-70 | Ecole Normale Supérieure de Jeunes Filles Montrouge, France |

*Operating system*: MVS JES2 (IBM-Pisa); MVS JES3 (IBM-Orsay)

*Programming language used*: FORTRAN IV

*High speed store required*: 872 K (IBM, Pisa); 248 K (IBM, Orsay)

*No. of bits in a word*: 32

*Peripherals used*: card reader, line printer, magnetic disc

*No. of cards in the program*: 800

*Keywords*: non-adiabatic, potential curves, projection, effective Hamiltonian, transition operator

*Nature of physical problem*
Determination of non-adiabatic potential surfaces from interaction configuration wavefunctions.

*Typical running time*
160 s for 6000 configurations (IBM-Pisa) (200 configurations only on IBM-Orsay and MODCOMP).

Computer Physics Communications 30 (1983) 169–175
North-Holland Publishing Company

# HEIZ – A PROGRAM TO ESTIMATE TEMPERATURE MODIFICATIONS IN LASER PLASMA INTERACTION EXPERIMENTS BY INVERSE BREMSSTRAHLUNG ABSORPTION AND CLASSICAL HEAT CONDUCTION

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Received 2 February 1983

## PROGRAM SUMMARY

*Title of program*: HEIZ

*Catalogue number*: ACES

*Computer*: CDC 175; *Installation*: Ruhruniversität Bochum

*Operating system*: NOS

*Programming language used*: FORTRAN 77

*High speed storage required*: 25.8 Kbytes

*No. of bits in a word*: 6

*Peripherals used*: card reader, line printer, plotter

*No. of cards in combined program and test deck*: 316

*Keywords*: laser–plasma interaction, inverse bremsstrahlung, heat conduction

*Nature of physical problem*
In order to overcome the lack of knowledge in laser plasma interaction experiments about the modification of an underdense plasma due to high power laser irradiation, a simple model was set up. The predictions of this model could be proved by several independent experiments [1–3]. The principal idea is that heating by inverse bremsstrahlung absorption is balanced by classical heat conduction out of the interaction zone.

*Method of solution*
Apart from an analytical recursion, only lowest order explicit Runge–Kutta methods are used for the solution of the corresponding differential equations [3].

*Restrictions on the complexity of the problem*
The 1-dimensional model assumes a homogeneous, extended plasma slab, and a homogeneous temperature distribution, before the laser is incident. The program is written for the $CO_2$-laser ($\lambda = 10.6$ μm). Parametric processes and further non-linear mechanisms are not taken into account. Electron quiver velocity should not exceed 6 times electron thermal velocity.

*Typical running time*
7.5 s for test run.

*Unusual features of the program*
If plots are wished, subroutine MALEN makes use of FOPLOT graphics commands. For different graphics systems, MALEN can easily be replaced by any user supplied plotting routine.

*References*

[1] B. Gellert, J. Handke and B. Kronast, Bull. Am. Phys. Soc. 26 (1981) 1000.
[2] B. Gellert and B. Kronast, 15th Eur. Conf. on Laser Interaction with Matter, Schliersee (Fed. Rep. Germany) (1982).
[3] J. Handke, SFB-report 82-N3-108, Ruhruniversität Bochum (1982).

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Computer Physics Communications 30 (1983) 177–185
North-Holland Publishing Company

# PROLATE RADIAL SPHEROIDAL WAVE FUNCTIONS

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Received 24 November 1982; in revised form 14 April 1983

## PROGRAM SUMMARY

*Title of program*: PRSWFN

*Catalog number*: ACEY

*Computer*: FELIX C-256; *Installation*: University Computer Centre, Cluj-Napoca, Romania

*Operating system*: SIRIS 2/3

*Programming language used*: FORTRAN IV

*High speed storage required*: 10 Kwords

*Number of bits in a word*: 32

*Peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 570

*Keywords*: general purpose, two-centre frame, radial spheroidal wave functions, expansion, Bessel functions

*Nature of physical problem*
The prolate radial spheroidal wave functions appear in a wide range of physical applications, and in particular in two-centre systems. The package PRSWFN contains six subprograms which compute these functions of both the first and second kind for any argument and accuracy.

*Method of solution*
The prolate radial spheroidal wave functions $R_{ml}^{(1,2)}(c, \xi)$ are calculated by summing spherical Bessel series, the coefficients being calculated separately, once for all the values of $\xi$; first the ratios of two consecutive coefficients are calculated recursively and then the final values of the coefficients are obtained through a normalization procedure [1].

*Restrictions on the complexity of the problem*
The package can be in principle applied to calculate any $R_{ml}^{(1,2)}(c, \xi)$. However, for high accuracy calculations of $R_{ml}^{(2)}(c, \xi)$ with $\xi$ close to unity and large $m$, the number of terms to be retained in the spherical Bessel series becomes very large, imposing large storage space and considerable computing time.

*Typical running time*
For $\xi = 1.077$, $c = 0.1$, ERRB $= 10^{-4}$ the number of terms in the $R_{ml}^{(2)}(c, \xi)$ series is 52. The run of this case took 7.7 s, from which about 90% of the time was dedicated to the calculation of the coefficients. The test run took about 9 min.

*Reference*

[1] C. Flammer, Spheroidal wave functions (Stanford Univ. Press, Stanford, 1957) (Russian translation, 1962).

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North-Holland Publishing Company

# PROLATE ANGULAR SPHEROIDAL WAVE FUNCTIONS

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Received 14 February 1983; in revised form 14 April 1983

## PROGRAM SUMMARY

*Title of program*: PASWFN

*Catalog number*: ACEZ

*Computer*: FELIX C-256; *Installation*: University Computer Centre, Cluj-Napoca, Romania

*Operating system*: SIRIS 2/3

*Programming language used*: FORTRAN IV

*High speed storage required*: 7 Kwords

*Number of bits in a word*: 32

*Peripherals used*: card reader, line printer

*Number of cards in combined program and test deck*: 494

*Keywords*: general purpose, two centre frame, angular spheroidal wave functions, associated Legendre functions

*Nature of the physical problem*
The prolate angular spheroidal wave functions are required in problems concerning the angular aspects of the solution of the Schrödinger equation in a two centre frame. The package PASWFN contains six subprograms which compute these functions of the first kind (the functions of the second kind are of minor physical interest) for any argument and accuracy.

*Method of solution*
The prolate angular spheroidal wave functions $S_{ml}(c, \eta)$ are calculated as series of associated Legendre functions of the first kind. The coefficients are calculated separately, for given values of $m$, $l$, $c$ [1], and are stored to be used in subsequent computations of $S_{ml}(c, \eta)$ for different values of $\eta$.

*Typical running time*
21 s for the test run.

*Reference*

[1] T.A. Beu and R.I. Câmpeanu, Comput. Phys. Commun. 30 (1983) 177.

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Computer Physics Communications 30 (1983) 193–205
North-Holland Publishing Company

# COMPUTATION OF TOTAL CROSS-SECTIONS FOR ELECTRON CAPTURE IN HIGH ENERGY COLLISIONS. II

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Received 14 March 1983

## PROGRAM SUMMARY

*Title of program*: CDW

*Catalogue number:* ACFA

*Computer:* IBM 3033; *Installation:* CNUSC, Montpellier (France)
The program has also been run on a PDP 11/45

*Operating system:* JES2

*Programming language used:* FORTRAN

*High speed storage required:* 80 Kwords

*Number of bits in a word:* 32

*Peripherals used:* input and output devices

*Number of cards in combined program and test deck:* 691

*Keywords:* atomic collisions, electron capture

*Nature of the physical problem*
Calculate the cross-section for electron-capture in high energy ion–atom collisions.

*Method of solution*
The program is based on the continuum distorted wave (CDW) method of Cheshire [1].

*Restriction on the complexity of the problem*
The present program is restricted to the case of fully stripped projectiles colliding with hydrogenic targets. The impact energy should be greater than 80 $\sup(|\epsilon_i|, |\epsilon_f|)$ keV/amu where $\epsilon_i$ and $\epsilon_f$ are the initial and final orbital energies of the captured electron expressed in atomic units.

*Typical running time*
The running time for the test run on the IBM 3033 is 5.98 s.

*Reference*

[1] I.M. Cheshire, Proc. Phys. Soc. 84 (1964) 89.

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* Equipe de recherche CNRS no. 260.

Computer Physics Communications 30 (1983) 207–217
North-Holland Publishing Company

# BAND STRUCTURE CALCULATIONS OF CUBIC METALS, ELEMENTARY SEMICONDUCTORS AND SEMICONDUCTOR COMPOUNDS WITH SPIN–ORBIT INTERACTION

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*Laboratory for Theoretical Physics, Boris Kidrič Institute for Nuclear Sciences, Belgrade, Yugoslavia*

Received 21 June 1982; in revised form 20 April 1983

## PROGRAM SUMMARY

*Title of program*: SPINORB

*Catalogue number*: ACKV

*Computer*: CDC-3600; *Installation*: Boris Kidrič Institute of Nuclear Sciences, Belgrade

*Operating system*: SCOPE 6,3

*Programming language used*: FORTRAN

*High speed storage required*: 43536 words

*No. of bits in a word*: 48

*Peripheral used*: CR

*No. of lines in combined program and test deck*: 1350

*CPC library subprograms used*: AAAF, AARC (included in deck)

*Keywords*: ***k***-space, energy bands, pseudopotential, spin–orbit interaction, solid state physics

*Nature of physical problem*
This work is concerned with the band structure calculations of metals, elementary semiconductors and semiconductor compounds with spin–orbit interaction included.

*Method of solution*
We applied the double expansion technique for the exact inclusion of the spin–orbit interaction influence in the band structure calculations of cubic metals, elementary semiconductors and semiconductor compounds. Our approach is based on the pseudopotential theory. The semiempirical variant of pseudopotential theory is the most successful in the description of electronic properties of crystals. In order to apply the double expansion technique it is necessary to solve the eigenvalue problem of one electron pseudo-Hamiltonian without spin–orbit interaction. For this, we use Brust's modification of Löwdin's perturbation technique [1]. The eigenfunctions obtained in this way have been used for the formation of new trial functions. After that, new trial functions have been applied for solving the eigenvalue problem of the Hamiltonian with spin–orbit term included, in the framework of the matrix method [2].

*Restrictions on the complexity of the problem*
Only applies to cubic metals, elementary semiconductors and semiconductor compounds.

*Typical running time*
About 40 min for test.

References

[1] D.R. Mašović and F. Vukajlović, Comput. Phys. Commun. 24 (1981) 181.
[2] G.C. Fletcher, The Electron Band Theory of Solids (North-Holland, Amsterdam-London, 1971) p. 34.

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Computer Physics Communications 30 (1983) 219
North-Holland Publishing Company

## ERRATUM NOTICE

*Title of paper*: A plotting package for visually comparing theoretical and experimental results
*Authors:*: J. Anderson, R.C. Beckwith, K.J.M. Moriarty and J. Tabor
*Reference:* Comput. Phys. Commun. 15 (1978) 437
*Title of adaptation*: POLAR PLOT AND IMPROVEMENTS
*Adaptation number*: 0001

Computer Physics Communications 30 (1983) 249–254
North-Holland Publishing Company

# MONTE CARLO SIMULATION OF PURE U($N$) AND SU($N$) GAUGE THEORIES ON A SIMPLICIAL LATTICE

J.-M. DROUFFE *
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Received 26 June 1983

## PROGRAM SUMMARY

*Title of program*: LATTICE

*Catalogue number*: ACFG

*Computer*: DEC VAX 11/780; *Installation*: Royal Holloway College Computer Centre

*Operating system*: DEC VAX 11/780: VMS 3.2

*Programming language used*: FORTRAN-77

*High speed storage required*: 110 Kwords

*Number of bits in a word*: 32

*Peripherals used*: terminal, line printer

*Number of lines in combined program and test deck*: 798

*Keywords*: lattice gauge theory, Yang–Millis theory, U($N$) and SU($N$) gauge theories, simplicial lattice, Wilson loops, Monte Carlo methods

*Nature of the physical problem*:
Lattice gauge theory is usually formulated on a hypercubical lattice [1]. However, in order to check universality it is necessary to formulate the theory on another lattice, e.g. the simplicial lattice [2]. The method for implementing the Monte Carlo algorithm for pure U($N$) and SU($N$) gauge theories on the recently introduced simplicial lattice is presented. The calculational technique for calculating all Wilson loops containing up to 13 triangles or 9 squares is explained.

*Method of solution*
Pure U($N$) and SU($N$) gauge theories are simulated by Monte Carlo methods on a four-dimensional simplicial space–time lattice. The method of Metropolis et al. [3] is used to equilibriate our lattice.

*Restrictions on the complexity of the program*
The only restriction on the program is the size of the links array which is dimensioned to

$$10(\mathrm{ISIZE})^4 \times 2N^2,$$

where ISIZE is the number of lattice sites in any space–time dimension and $N^2$ is the number of elements in an U($N$) or SU($N$) matrix. This effectively sets the limit to the size of lattice which will reside in real memory. Of course, the VAX 11/780 is a virtual memory machine and we could use this facility to examine larger lattices.

*Typical running time*
The test run took 6 h and 17 min on the VAX 11/780 with ISIZE = 6 and $N = 2$ for 42 sweeps through the lattice.

*References*

[1] K.G. Wilson, Phys. Rev. D10 (1974) 2455.
[2] J.-M. Drouffe and K.J.M. Moriarty, Nucl. Phys. B220 (FS8) (1983) 253.
[3] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller and E. Teller, J. Chem. Phys. 21 (1953) 1087.

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Computer Physics Communications 30 (1983) 255–257
North-Holland Publishing Company

# IMPLEMENTATION OF THE MICROCANONICAL MONTE CARLO SIMULATION ALGORITHM FOR SU($N$) LATTICE GAUGE THEORY CALCULATIONS *

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and

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Received 30 June 1983; in revised form 11 July 1983

## ADAPTATION SUMMARY

*Title of adaptation*: MICROCANONICAL DEMON

*Adaption number*: 0001

*Reference to original program*:

*Title of program*: SUUNFA

*Catalogue number*: AAOT

*Ref. in CPC*: 29 (1983) 97

*Authors of original program*: R.W.B. Ardill, K.J.M. Moriarty and Michael Creutz

*High speed store required*: 47 Kwords

*No. of bits in a word*: 64

*Additional keywords*: microcanonical demon

*Number of cards required to effect adaptation (including directive cards)*: 20

*Nature of the physical problem*
Recently a new algorithm for Monte Carlo simulation, called the microcanonical algorirthm [1], was introduced for lattice gauge theory calculations. We wish to apply this technique to SU(3) gauge theory.

*Method of solution*
We altered a previously introduced Monte Carlo simulation program [2] to implement the microcanonical algorithm for SU(3) gauge theory [3].

*Restrictions on the complexity of the program*
The only restriction on the complexity of the program is the size of gauge field links array. This array, called ALAT, must be adjusted to fit the memory of the computer available to the user.

*Typical running time*
To generate the test run output took about 1 h 23 min of CRAY-1S CPU time.

*References*

[1] M. Creutz, Phys. Rev. Lett. 50 (1983) 1411.
[2] R.W.B. Ardill, K.J.M. Moriarty and M. Creutz, Comput. Phys. Commun. 29 (1983) 97.
[3] M. Creutz and K.J.M. Moriarty, Microcanonical Monte Carlo Simulation of SU(3) Gauge Theory in Four Dimensions, Brookhaven National Laboratory Preprint (June 1983).

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* Part of this paper has been written under contract DE-AC02-76CH00016 with the US Department of Energy.

Computer Physics Communications 30 (1983) 259–269
North-Holland Publishing Company

# A PROGRAM FOR PERSPECTIVE VIEWS OF OPEN SURFACES

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Received 11 May 1983

## PROGRAM SUMMARY

*Title of program*: TDPLOT3

*Catalogue number*: ACFB

*Computer*: IBM 3081. IBM 370, IBM 360; *Installation*: TUCC, Research Triangle Park, NC 27709, USA

*Operating system*: OS/370, MVS

*Program language used*: IBM Fortran H (code compatible with ANS Fortran except for minor extensions)

*High speed storage required*: compilation 266 Kwords, link edit 49 Kwords, execution 66 Kwords

*No. of bits in a word*: 32

*Peripherals used*: line printer, multi-color or single color plotter

*No. of cards in combined program and test deck*: 5493

*Keywords*: perspective projection, computer display, stereoscopy, cylindrical coordinates, spherical polar coordinates, plotting, hidden-line removal

*Nature of the physical problem*
TDPLOT3 constructs either monoptic or stereoptic perspective projections of open surfaces described in spherical polar or cylindrical coordinates and, optionally, displays the top side of the surface in one color and the underside in another color.

*Method of solution*
TDPLOT3 scales the surface so that its projection fits within the specified plot dimensions. It then constructs the perspective projection of the surface, determines which points in the projection are hidden, and, finally, plots the projection with hidden lines removed.

*Restrictions on the complexity of the problem*
TDPLOT3 generates perspectives of surfaces $s(r,\theta)$ parametrized in spherical polar or cylindrical coordinates where the radial, $r$, and the angular, $\theta$, variables are tabulated in uniform steps. The function $s(r,\theta)$ must be single valued, and no part of the display plane on which the surface is projected, when extended to infinity, should intersect the surface.

*Typical running time*
The time estimates presented here are in equivalent IBM 3081 CPU time (about 0.8 μs per arithmetic operation). For a typical surface comprising 49 radial by 40 angular points the CPU time required for constructing three different perspectives (two monoptic and one stereoptic) is approximately 3.1 s, with additional time required for output.

*Unusual features of the program*
TDPLOT3 offers three different types of hidden-line elimination, two of which have been described previously [1]. In the third type, lines visible on the top side of the surface are distinguished from those visible on the underside so that a display may be constructed with the perspective of the top side of the surface in one color and the perspective of the underside in another color. TDPLOT3 also features a cubic-interpolation routine which generates additional perspective points so that a smoother display of the surface may be constructed without needing additional input data or hidden-line search time [1]. Monoptic and various types of stereoptic views can be produced [1]. The program structure is modular; consequently, those subroutines which are necessary for multi-color plotting may be removed when only single color plotting capabilities are available. Standard ASA FORTRAN 77, compatible with ASA FORTRAN 66, is used except for subroutines which drive the plotter.

*Reference*
[1] E.A. Olszewski and W.J. Thompson, Comput. Phys. Commun. 21 (1980) 185, and references cited therein.

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Computer Physics Communications 30 (1983) 271–275
North-Holland Publishing Company

# PARAMETRIZATION OF THE BAND STRUCTURE OF FCC CRYSTALS

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Received 1 July 1982; in revised form 4 May 1983

## PROGRAM SUMMARY

*Title of the program*: BAPAR

*Catalogue number*: ACKU

*Computer*: CYBER 170-720; *Installation*: Ecole Polytechnique Federal, Lausanne

*Operating system*: NOS.BE

*Programming language used*: FORTRAN

*High-speed storage required*: 14000 words

*No. of bits in a word*: 60

*Peripherals used*: card reader, line printer

*No. of lines in combined program and test deck*: 445

*Keyword*: band structure interpolation

*Nature of the physical problem*
The program fits the energy bands of fcc crystals.

*Method of solution*
The method consists in treating the integrals contained in the Hamiltonian matrix as independent parameters. With a starting set of approximated values of these integrals, the program evaluates the eigenvalues of the Hamiltonian matrix and calculates the mean value of the difference between them and the energy values of the bands to be fitted. The user has to give a limit to this difference; the program modifies the parameters until this limit is reached, finding at the ened of the iterations the "best estimate" set of parameters which fits the true band.

*Typical running time*
60–70 s.

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Computer Physics Communications 30 (1983) 277–299
North-Holland Publishing Company

# ABACUS: A NATURAL LANGUAGE FOR THE NUMERICAL COMPUTATION OF MATHEMATICAL FORMULAE

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Received 26 July 1982; in revised form 6 June 1983

## PROGRAM SUMMARY

*Title of program:* ABACUS

*Catalogue number:* ACFC

*Computer*: VAX 11-780; *Installation:* Istituto Nazionale di Fisica Nucleare – Centro Nazionale Analisi Fotogrammi – Via Mazzini 2, 40138 Bologna Italy

*Operating system:* VMS

*Programming language used:* FORTRAN 77

*Number of bits per word:* 32

*Peripherals used:* video terminal, line printer

*Number of cards in combined program and test deck:* 3759

*Nature of physical problem*
The program allows interactive computation of mathematical formulae, iterative procedures and metric conversions.

*Method of solution*
Parsing of input string and use of basic mathematical functions as supported by the language itself.

*Restriction on the complexity of the problem*
The limits are set to fit the mainly interactive use of the program.

*Typical running time*
No running time measure is considered as the use is mainly interactive and the limit is set by the user himself, the result appearing on VT immediately after the input formula is typed.

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Computer Physics Communications 30 (1983) 301–309
North-Holland Publishing Company

# A PROGRAM TO GENERATE THE SYMMETRY-ADAPTED ROTATIONAL EIGENFUNCTIONS AND ENERGY LEVELS FOR ASYMMETRIC TOP MOLECULES

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Received 16 December 1982

## PROGRAM SUMMARY

*Title of program*: ASYMTOP

*Catalogue number:* ACFD

*Computer*: VAX 11/780; *Installation*: The Queen's University of Belfast

*Operating system*: VMS

*Programming language used*: FORTRAN IV

*High speed storage required*: 3607

*No. of bits in a word*: 32

*Peripherals used*: line printer, card reader, card punch (optional)

*No. of lines in combined program and test deck*: 852

*NAG-LIBRARY subroutines used*: F02ABF and M01AJF (for ref. see inside)

*Keywords*: symmetry operation. rotational eigenfunction, energy levels, asymmetric top, irreducible representation, moment of inertia, point group, Eulerian angles, space-fixed axes, molecule-fixed axes, angular momentum

*Nature of physical problem*
Symmetry-adapted rotational eigenfunctions and energy levels are generated using symmetry properties of an asymmetric top molecule for any given value of the angular momentum quantum number $J$.

*Method of solution*
The rotational eigenfunctions of an asymmetric top are expanded in terms of symmetry-adapted symmetric top functions. The total Hamiltonian matrix of the rotational motion of the molecule is split into four submatrices according to the point group properties of the asymmetric top. The resulting secular equations corresponding to each irreducible representation (IR) of the point group are solved as usual to give eigenvalues and eigenvectors. These eigenvalues (energy levels) and eigenvectors (expansion coefficients) are then classified according to their IR and the submatrix.

*Restriction on the complexity of the problem*
The program can take $J$ up to 7, but for $J > 7$, the program can easily be modified.

*Typical running time*
About 2 s for $J = 4$ (IJ = 1) on VAX11/780 system.

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* Present address: Joint Institute for Laboratory Astrophysics, The University of Colorado and National Bureau of Standards, Boulder, CO 80309, USA.

Computer Physics Communications 30 (1983) 311–323
North-Holland Publishing Company

# AN ATOMIC GAUSSIAN-TYPE ORBITAL ROOTHAAN–HARTREE–FOCK PROGRAM

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and

Y. SAKAI

*College of General Education, Kyushu University, Ropponmatsu, Fukuoka, Japan*

Received 29 April 1983

## PROGRAM SUMMARY

*Title of program*: HSCF

*Catalogue number*: AAFI

*Computer for which the program is designed and others on which it is operable*: Amdahl 5860, IBM 360, IBM 370

*Computer*: Amdahl 5860; *Installation*: Computing Services, University of Alberta, Edmonton, Alberta

*Operating system*: MTS

*Programming language used*: FORTRAN IV

*High speed storage required*: 327 164 words

*No. of bits in a word*: 32

*Peripherals used*: card reader, line printer

*No. of lines in combined program and test deck*: 2393

*CPC Library subprograms used*: subroutine CARDIN from program MCDF, *Cat. no.*: AANC; *Ref. in CPC*: 21 (1980) 207

*Keywords*: atomic, SCF, Roothaan–Hartree–Fock method, Gaussian-type orbitals, complex atoms, Gaussian basis sets for molecular calculations

*Nature of physical problem*
The non-relativistic Roothaan–Hartree–Fock equations are set up and solved using an analytical basis of Gaussian-type orbitals. This provides atomic total energies and orbital energies in a given basis set which may be further used in analyzing results obtained in molecular calculations using the same basis set.

*Method of solution*
The self-consistent-field equations for an atom in a general open-shell state are set up following the method of Roothaan [1]. Electrostatic interactions in a given state are defined via vector coupling constants whose numerical values were published for all the states accessible to the HSCF program [1,2]. The method used allows for several open-shells in an atom but not more than one open-shell for each symmetry species.

*Restrictions on the complexity of the problem*
The present version of the program is restricted to four symmetry species, 18 basis functions per symmetry species, 11 primitive Gaussian functions per contracted Gaussian-type orbital. Restrictions on many arrays depend on the actual combination of the number of symmetry species and the number of basis orbitals used for each species. The restrictions are fully described in comment cards in subroutine DATA.

*Unusual features of the program*
1. IMPLICIT statement;
2. End-of-file condition is detected using END = construct (subroutine DATA);
3. Array names (not array elements) are used to define initial

values of array elements (DATA statements);

4. Length specification in FUNCTION statements (FUNCTION'S JSM, KSM);
5. An asterisk as a dummy argument; statement number as an actual argument; RETURN *i* statement is used (subroutine SCF);
6. Arithmetic expressions are used as subscript expressions in WRITE lists.

*References*

[1] C.C.J. Roothaan and P.S. Bagus, in: Methods in Computational Physics, Vol. II, eds. B. Alder, S. Fernbach and M. Rotenberg, (Academic Press, New York, 1963) p. 47.

[2] G.L. Malli and J.P. Olive, in: Technical Report of the Laboratory of Molecular Structure and Spectra, Dept. of Physics, University of Chicago (1962–1963) Part 2, p. 258.

Computer Physics Communications 30 (1983) 325–331
North-Holland Publishing Company

# DETERMINATION OF ANTIGENIC DETERMINANTS

Serafin FRAGA

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Received 6 June 1983

## PROGRAM SUMMARY

*Title of program*: DIAD

*Catalogue number*: ACFH

*Computer for which the program is designed and others on which it is operable*: Amdahl 580/5860 and IBM-type computers

*Computer*: Amdahl 580/5860; *Installation*: University of Alberta Computing Services

*Operating system*: MTS

*Programming language used*: Fortran IV

*High speed storage required*: 10 kwords

*No. of bits in a word*: 32

*Peripherals used*: disks, printer

*No. of lines in combined program and test deck*: 820

*Keywords*: proteins, antigenic determinants, vaccines

*Nature of the physical problem*
Determination of the sequence positions of the probable antigenic determinants in a protein.

*Method of solution*
The prediction of the sequence positions of the antigenic determinants is based on the characteristics of the hydrophilicity and recognition profiles of the protein under study.

*Restrictions on the complexity of the problem*
Only proteins involving the amino acids ala, arg, asn, asp, cys, glu, gln, gly, his, ile, leu, lys, met, phe, pro, ser, thr, trp, tyr and val (as well as hydroproline) may be studied. The amino acid sequence of the protein must be known.

*Typical running time*
0.1 s for the test run (with three cases).

*Unusual features of the program*
This program has been prepared from a version, in operation at the University of Alberta, which produces the graphical representations of the hydrophilicity, recognition and composite profiles for the protein under study. The plotting subroutines, available at the institution where the program will be run, may be used for this purpose.

*Reference*

[1] S. Fraga, Can. J. Chem. 60 (1982) 2606.

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Computer Physics Communications 30 (1983) 359–368
North-Holland Publishing Company

# PFPOSFIT: A NEW VERSION OF A PROGRAM FOR ANALYSING POSITRON LIFETIME SPECTRA WITH NON-GAUSSIAN PROMPT CURVE

Werner PUFF

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Received 8 July 1982; in final form 12 July 1983

## PROGRAM SUMMARY

*Title of program*: PFPOSFIT

*Catalogue number*: ACKX

*Computer*: UNIVAC 1100/81; *Installation*: Technical University of Graz

*Programming language used*: FORTRAN 77

*High speed storage required*: data: 5939 IBANK, 44275 DBANK

*No. of bits in a word*: 36

*Overlay structure*: yes

*No. of lines in combined program and test deck*: 3312

*References to other published versions of this program*:

| *Cat. No.* | *Title* | *Ref. in CPC* |
|---|---|---|
| AAGK | POSITRONFIT | 3(1972)240 |
| AAGX | POSITRONFIT EXTENDED | 7(1974)401 |
| AAGZ | DBLCON | 13(1978)371 |
| AAHI | INTERACTIVE POSITRONFIT | 15(1978) 97 |
| AANN | PATFIT | 23(1981)307 |

*Keywords*: positron annihilation, lifetime, time spectrum, least-squares, fitting, convolution, minimization, sum-of-exponentials, Marquardt, constraints, correlation matrix

*Nature of the physical problem*
A measured positron lifetime spectrum consists of a sum of exponential decay components smeared with the instrumental resolution function. Experimenters want to extract the lifetimes and intensities of the different components.

*Method of solution*
Positron lifetime spectra are analyzed by a semilinear least-squares technique.

*Restriction on the complexity of the program*
Five lifetime components, two exponentials in the prompt, 512 channels in the spectrum.

*Typical running time*
The test run requires about 31 s CPU time on the UNIVAC 1100/81.

Computer Physics Communications 30 (1983) 369–381
North-Holland Publishing Company

# AMPLITUDES FOR SCATTERING OF ELECTRONS BY ATOMIC SYSTEMS INCLUDING RELATIVISTIC EFFECTS

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*Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast BT7 1NN, N. Ireland*

Received 22 January 1983

## PROGRAM SUMMARY

*Title of program:* SCATTAMPREL

*Catalogue number:* ACFE

*Computer:* VAX 11/780; *Installation:* The Queen's University of Belfast, Belfast, Northern Ireland

*Operating system:* VMS V3.0

*Programming language used:* FORTRAN 77

*High speed storage required:* 69056 words

*Number of bits in a word:* 64

*Peripherals used:* card reader, line printer

*Number of lines in combined program and test deck:* 1247

*Key words:* atomic, scattering, reactance matrix, transition matrix, elastic, inelastic, superelastic, scattering amplitudes, electron, heavy atoms, noble gases, relativistic effects, spin–orbit interaction, *JlK*-coupling scheme

*Nature of physical problem*
SCATTAMPREL calculates scattering amplitudes for the electron–atom scattering process. The scattering amplitudes provide all possible information about the scattering process.

*Method of solution*
Given *K*- or *T*-matrices, calculated in the *JlK*-coupling scheme [1,2], SCATTAMPREL determines the corresponding scattering amplitudes using a relationship derived according to the method of Blatt and Biedenharn [3].

*Restrictions on the complexity of the program*
In its present form SCATTAMPREL only calculates scattering amplitudes for electrons scattering from neutral atoms.

*Typical running time*
Test run I took 2.38, test run II took 2.54 s execution time on the VAX 11/780.

*References*

[1] N.S. Scott and K.T. Taylor, Comput. Phys. Commun. 25 (1980) 347.
[2] H.E. Saraph, Comput. Phys. Commun. 3 (1972) 256.
[3] J.M. Blatt and L.C. Biedenharn, Rev. Mod. Phys. 24 (1952) 258.

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Computer Physics Communications 30 (1983) 383–396
North-Holland Publishing Company

# PROGRAM TO CALCULATE OBSERVABLE QUANTITIES FROM SCATTERING AMPLITUDES FOR INELASTIC ELECTRON–ATOM COLLISIONS

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Received 22 January 1983

## PROGRAM SUMMARY

*Title of program*: OBSERVABLES

*Catalogue number*: ACFF

*Computer*: VAX 11/780; *Installation*: The Queen's University of Belfast, Belfast, Northern Ireland

*Programming language used*: FORTRAN 77

*Operating system*: VMS V3.0

*High speed storage required*: 20864 words

*Number of bits in a word*: 32

*Peripherals used*: card reader, line-printer

*Number of lines in combined program and test deck*: 1458

*Keywords*: inelastic, electron–atom scattering, differential cross-section, spin polarization, scattering asymmetry, alignment, orientation, spin–orbit interaction, perturbation coefficients, atomic, scattering

*Nature of physical problem*
For inelastic electron–atom scattering; the cross-section, spin polarisation; scattering asymmetry, alignment and orientation parameters; angular distribution and polarisation of the emitted light in electron–photon coincidence experiments are calculated.

*Restrictions on the complexity of the problem*
Parts of the program (underlined twice in the flow diagram) may only be used for $J = 0$, even → $J = 1$, odd (or $L = 0$, even → $L = 0$, odd) transitions.

*Typical running time*
The test run took 2.73 s execution time on the VAX 11/780.

Computer Physics Communications 30 (1983) 397–402
North-Holland Publishing Company

# FASTF: FAST FOURIER TRANSFORM WITH ARBITRARY FACTORS

Eduardo GARCIA-TORAÑO

*Metrología, Edificio 3, Junta de Energía Nuclear, Avenida Complutense 22, Madrid-3, Spain*

Received in final form 15 June 1982

## PROGRAM SUMMARY

*Title of program*: FASTF

*Catalogue number*: ACUH

*Computer*: UNIVAC 1100/81; *Installation*: Centro de Cálculo, Junta de Energía Nuclear

*Operating system*: EXEC 8

*Programming language used*: FORTRAN IV

*High speed storage required:* 8 kwords for the test run

*No. of bits in word*: 36

*Peripherals used*: card reader, line printer

*No. of cards in combined program and test deck*: 376

*Keywords*: fast Fourier transform, Fourier, time series analysis

*Nature of the problem*
FASTF performs a discrete Fourier transform (direct/inverse) of a complex vector of length $N$. $N$ should be factorisable as $N = r_1 r_2 \dots r_p$ ($r_i$ integers).

*Method of solution*
The fast Fourier transform algorithm as described in ref. [1].

*Restrictions on the complexity of the problem*
The lowest $r_i$ should be less than 181 for storage limitations. This condition may be modified by increasing the size of the IPRIM array which contains a list of the 40 first prime numbers.

*Typical running time*
The execution time depends on $N$. A set of 1024 points is transformed in 0.544 s.

*Reference*
[1] W.T. Cohram et al., IEEE Trans. on Audio and Electroacoustics AU-15 (1967) 45.

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Computer Physics Communications 30 (1983) 403–409
North-Holland Publishing Company

# A MODIFICATION TO PLATTSUM, A PROGRAM THAT EVALUATES ELECTROSTATIC LATTICE SUMS BY THE PLANEWISE SUMMATION METHOD

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*División de Física del Solido, Comisión Nacional de Energía Atómica, Avenida del Libertador 8250, 1429 Buenos Aires, Argentina*

Received 8 July 1982

## PROGRAM SUMMARY

*Title of the program: PLATTSUM2*

*Catalogue number*: ACKW

*Computer*: IBM 370/158; *Installation*: Comisión Nacional de Energía Atómica, Av. del Libertador 8250, 1429 Buenos Aires, Argentina

*Operating system*: OS/VS1 or VM370/CMS

*Programming language used*: FORTRAN IV

*High speed storage required*: 67984 bytes

*No. of bits in a word*:32

*Peripherals used*: card reader, line printer and/or on-line terminal

*No. of cards in combined program and test deck*: 1557

*Keywords*: lattice sums, crystal field, Lorentz factor, electrostatic crystal energy, Ewald potential, planewise summation method

*Nature of physical problem*
The input and output of the program PLATTSUM [1] for evaluating electrostatic lattice sums have been modified in such a way as to reduce the manual work of the user when the calculation involves many field points and/or many source sublattices.

*Method of solution*
The computer is fed with the coordinates of the field points and sublattice sites and is directed to calculate the required lattice sums for a specified set of field points and sublattices. All the relative coordinates between field and source points are evaluated by the program itself.

An additional output has been provided, where the results are tabulated so as to be used as input for another program.

*Restriction on the complexity of the problem*
Same as for PLATTSUM. Number of field points and source sublattices not greater than 200. This restriction can be easily relaxed.

*Typical running time*
For each pair field point-source sublattice the running time is the same as for each data set of PLATTSUM.

*Unusual features of the program*
Same as for PLATTSUM.

*Reference*

[1] J.A. Hernando and V. Massidda, Comput. Phys. Commun. 22 (1981) 13, erratum: 25 (1982) 111.

Computer Physics Communications 30 (1983) 411–419
North-Holland Publishing Company

# SOLITON BAG MODEL

Rudolf SALY

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Received 5 July 1983

## PROGRAM SUMMARY

*Title of program:* SOLITON

*Catalogue number:* AAVQ

*Computer:* VAX-11/780; *Installation:* NRC-High Energy Physics, Carleton University

*Operating system:* VAX/VMS

*Programming language used:* FORTRAN 77

*High speed storage required:* 40 000 words, can vary

*No. of bits in a word:* 32

*Peripherals used:* line printer, card reader

*No. of cards in combined program, test deck and description:* 550

*Keywords*: particle physics, nonlinear differential equations, soliton, bag model, Dirac equation

*Nature of physical problem*
The soliton bag model is a generalization of the MIT and SLAC bag models [1]. Mathematically the problem equals to boundary and eigenvalue problems for a system of coupled linear ordinary differential equations, integral equations and a nonlinear differential equation. The calculated quantities include: quark energy, bag energy, total hadron energy, magnetic moment, charge radius, ratio of axial-vector/vector coupling, etc.

*Method of solution*
The problem is solved by iteration whose cycle involves the following three steps:

1) solution of the radial Dirac equations (eigenvalue problem),
2) renormalization of the quark wave functions,
3) solution of the nonlinear differential equation by the Newton method (two point boundary value problem).

The main tool in all three steps is a direct Taylor series expansion of the functions involved. The boundary (eigenvalue) problems are solved using a shooting method based on bi-section and parabola iteration.

*Typical running times*
Execution of the program in the test case (accuracy 0.5% or 12 iterations) takes 1 min on the VAX-11 computer.

*Reference*

[1] T.D. Lee, Particle Physics and Introduction to Field Theory (Harwood Academic, New York, 1981) chap. 20.

Computer Physics Communications 30 (1983) 421–428
North-Holland Publishing Company

# WILSON LOOPS, STRING TENSION AND CORRELATIONS IN MONTE CARLO SIMULATION OF COMPACT $U(1)$ LATTICE GAUGE THEORY

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Received 9 July 1983

## PROGRAM SUMMARY

*Title of program*: LATT

*Catalogue number*: ACFJ

*Computer*: DEC VAX 11/780; *Installation*: Royal Holloway College Computer Centre

*Operating system*: DEC VAX 11/780: VMS 3.2

*Programming language used*: FORTRAN-77

*High speed storage required*: 16 Kwords

*No. of bits in a word*: 32

*Peripherals used*: card reader, line printer

*Total no. of lines in combined program and test deck*: 1301

*Keywords*: lattice gauge theory, $U(1)$, quark confinement, phase diagram, phase transition, statistical mechanics, average action per plaquette, Monte Carlo simulation, Wilson loop, string tension, correlations

*Nature of the physical problem*
The program calculates Wilson loops, their correlations and the string tension for $U(1)$ lattice gauge theory. These are useful observables [1] for studying the phase structure of $U(1)$ lattice gauge theory.

*Method of solution*
Monte Carlo techniques are used to generate a series of field configurations of the lattice system at a given temperature. For each configuration the Wilson loops are calculated, the string tension extracted and, if desired, correlations between the loops are evaluated. The program uses the technique of sweeping through the lattice described in ref. [2].

*Restrictions on the complexity of the program*
The storage required is dependent on the lattice size. The execution time increases with the lattice size and with the number of Monte Carlo iterations required, and is typically rather long. At temperatures much below the critical point, the Monte Carlo vetoing process becomes very slow.

*Typical running time*
The test run took 13.5 s on the DEC VAX 11/780.

*References*
[1] K.G. Wilson, Phys. Rev. D10 (1974) 2455.
[2] R.C. Edgar, L. McCrossen and K.J.M. Moriarty, Comput. Phys. Commun. 22 (1981) 433.

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## APPLICATION FOR A SUBSCRIPTION TO THE PROGRAM LIBRARY

A description of the Library Services is given in Comput. Phys. Commun. 19 (1980) 11–15. A summary is given on the preceding pages.

Name of person authorising the subscription
Name of institute
Address
Type of computer

*Magnetic tape specification:*

The library programs will be sent as card images on magnetic tape without a header label. Please indicate, by ticking the appropriate boxes, the mode in which the tape should be written. Please specify the requirements if the alternatives given are impossible.

| | | | |
|---|---|---|---|
| Magnetic tape width: | $\frac{1}{2}$-inch ☐ | | |
| Number of tracks: | 9-track ☐ | other ☐ | |
| Density: | 800 characters ☐ per inch | 1600 characters ☐ per inch | other ☐ |
| Parity: | even ☐ | odd ☐ | |
| Inter-block gap: | 0.6 inch ☐ | other ☐ | |

Number of card images per block (block length = $80n$ characters, $n \leqslant 24$).

*Character code:*

The most common code on 9-track tape is odd parity EBCDIC. If this is unsuitable please define the code required.

*Subscription charge:*

The subscription for 1985 is £175 per volume plus the cost of a tape and its postage.

Please return to:
Miss C. Jackson
CPC Program Library
Department of Applied Mathematics and Theoretical Physics
Queen's University of Belfast
Belfast BT7 1NN
Northern Ireland

Signed:

Address:

Date:

Neither the Library nor the Author of any distributed program guarantees that it is free from error or meets its published specification and cannot be responsible for any loss or consequential damage as a result of using it.

The subscriber will be asked to limit the distribution of the programs in the Library to authorized users of the facilities provided by his institution.

1985

## C.P.C. PROGRAM LIBRARY-ORDER FORM

A description of the Library Services is given in Comput. Phys. Commun. 19 (1980) pp. 11–15.

Please list the program(s) required. Kindly check whether any program calls other C.P.C. Library subprograms since these should also be listed.

| | | |
|---|---|---|
| Catalogue number | Title | No. of cards |
| Type of computer: | | Total no. of cards |

*Magnetic tape specification:*

The library programs will be sent as card images on magnetic tape without a header label. Please indicate, by ticking the appropriate boxes, the mode in which the tape should be written. Please specify the requirements if the alternatives given are impossible.

| | | | |
|---|---|---|---|
| Magnetic tape width: | $\frac{1}{2}$ ☐ | | |
| Number of tracks: | 9-track ☐ | other ☐ | |
| Density: | 800 characters ☐ per inch | 1600 characters ☐ per inch | other ☐ |
| Parity: | even ☐ | odd ☐ | |
| Inter-block gap: | 0.6 inch ☐ | other ☐ | |

Number of card images per block (block length = $80n$ characters, $n \leqslant 24$).

*Character code:*

The most common code on 9-track tape is odd parity EBCDIC. If this is unsuitable please define the code required.

*Charge:*

For 1985 this is £10 per 1000 card images plus a basic charge of £20. This includes the cost of a tape (maximum length 600 ft. (180 m)), handling and air-mail postage.

*Program listings:*

If a magnetic tape is not suitable, listings can be supplied. In 1985, the charge for listings is £2 per 1000 lines plus a basic charge of £10. Postage is charged extra. Please specify if listings are required.

*Method of ordering:*

If an official order from requestor's institute is also enclosed the order will be dispatched immediately. Otherwise a proforma invoice will be issued. The programs will then be dispatched when this invoice is returned with the remittance. All payments should be made in sterling.

Please return to:
Miss C. Jackson
CPC Program Library
Department of Applied Mathematics
Queen's University of Belfast
Belfast BT7 1NN
Northern Ireland

Signed:

Address:

Date:

Neither the Library nor the Author of any distributed program guarantees that it is free from error or meets its published specification and cannot be responsible for any loss or consequential damage as a result of using it.

The requestor will be asked to limit the distribution of the program(s) to members of his group.

# Les Houches 1985
# XLV

## Summer School

# SIGNAL PROCESSING

12 August - 6 September 1985

Time series analysis, Random functions. Detection and Estimation theory. Linear and non linear filtering, parametric and non parametric representations. Time frequency representation. Artificial intelligence in signal processing. Adaptive systems. Spectrum estimation. Digital signal processing. Image processing and reconstruction. Array processing. Time delay estimation. Architecture of Signal processing systems. Fast algorithms for signal processing. This session intends to offer a synthetic presentation of the state of art in Signal Processing from the most recent developments of theoretical backgrounds to the most important fields of applications and the new technical aspects in system and algorithm design. The aim of the session is to allow specialists of all the areas of Signal Processing to get a clear and global view of the new challenging problems faced by the current development of signal processing taking into account the simultaneous growth of fundamental discoveries, the impulsive effects of users applications and of new hardware and software technologies. S. Kay, V. Cappellini, G.C. Carter, C. Gueguen and others will contribute to enlighten the new frontiers in this fast growing field.

## MAIN LECTURERS

**J.F. Boehm, V. Cappellini, G.C. Carter, T.S. Durrani, Y. Grenier, C. Gueguen, T. Kailath, S. Kay, S.Y. Kung, B. Picinbono, S. Reddaway, L. Scharf, A. Venetsanopoulos, G. Kopec, W.F.G. Mecklenbrauker, to be confirmed.**

## ORGANIZATION

The Summer School of Les Houches is an institute affiliated with the Grenoble University.
This session is under consideration by the Scientific Affairs Division of NATO.
The Scientific Directors are T.S. Durrani, J.L. Lacoume.

Established in 1951, the School is located in a group of mountain chalets surrounded by meadows and woods, in the French Alps near Chamonix, facing the Mont-Blanc.

Accommodation and meals are provided within the School for both participants and lecturers.

## APPLICATIONS

Additional information and application forms may be obtained from:
**Ecole d'Eté de Physique Théorique, 74310 Les Houches, France**
Posters available upon request.

## DEADLINE

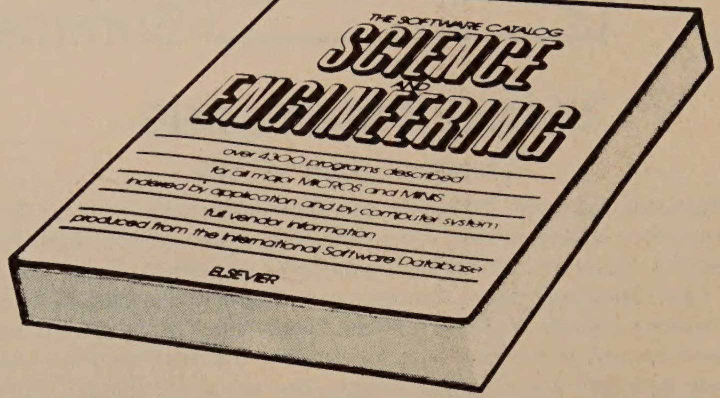
Applications and letters of recommendation must have reached the School *by 1 March 1985*

*The first 1985 session will be entitled Architecture of Fundamental Interactions at Short Distances*

*Two sessions will be held in 1986, one on Disordered Systems, the other on the Physics of strongly Ionized Atoms.*

P152NH

# ANNOUNCING
## The Complete Software Reference for Scientists and Engineers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Designed specifically for scientists and engineers, this timesaving reference is your guide to information on availability, price, applications, and compatibility of more than 4,300 existing micro- and minicomputer packages and the systems they run on. Every listing has been chosen for its use and applicability to the science and engineering fields; every effort has been made to eliminate programs of marginal interest.

**The Software Catalog: Science and Engineering** is the most comprehensive, most completely cross-referenced directory of its type. Use its unique indexing system to find software from any of these reference points: vendor, computer system, operating system, programming language, microprocessor, application, and keyword.

**Lists software in these categories:**

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- CAM – Computer Aided Manufacturing
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- Engineering (Electrical and Electronic)
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- Engineering (Other)
- Manufacturing
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SCIENTIFIC
- Astronomy
- Biology
- Chemistry
- Earth Science
- Environmental Science
- Mathematics
- Nuclear Science
- Physics
- Statistics

PROFESSIONS/INDUSTRIES
- Aerospace
- Agriculture
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- Automotive Industry
- Aviation
- Chemical Industry
- Energy (Oil, Gas, Alternatives, Etc.)
- Medicine/Dentistry
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- Transportation

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NH112

# COMPUTER PHYSICS COMMUNICATIONS INSTRUCTIONS TO AUTHORS *

## (ABBREVIATED VERSION)

Two classes of papers are published by Computer Physics Communications:

(i) Papers in the general area of computational physics including review articles, conference proceedings, research papers, notes and letters.

(ii) Write-ups describing programs to be held in the CPC International Physics Program Library † together with program adaptations and erratum notices.

Upon acceptance of an article, the author(s) will be asked to transfer copyright of the article to the publisher. This transfer will ensure the widest possible dissemination of information.

### Computational physics papers

Papers for inclusion in CPC should not primarily be concerned with theoretical or experimental physics or with mathematics, computer science or information engineering but should be specifically relevant to computational physics and quantum chemistry or to the computing needs of the physics community. Subject to this criterion CPC will publish descriptions of:

Numerical, computational and programming methods.
Software, hardware and network techniques and facilities.
Mathematical, graphical and other subroutine libraries used in physics.
Programs in a particular field of physics or quantum chemistry.
Methods and programs associated with the design, running or analysis of experiments.
Languages and system programs of particular importance to physicists or quantum chemists,

together with comments on manufacturers' hardware and software and on previous publications in CPC.

### Computer programs in physics

The programs described should be of use to other physicists or illustrate new programming techniques which are of importance to some branch of computational physics. Since they are intended for general application within the physics community they should be well structured, laid out and documented with sufficient tables and comments to make their working clear. They should be written either in USANS FORTRAN IV, FORTRAN 77 or ALGOL 60, or in some other language which has been adequately standardized and described in the literature and whose compiler is sufficiently widely available. Dialect statements and systems or library subroutines which are restricted to a particular manufacturer or installation should be avoided.

### Submission of manuscripts

Letters should be submitted to the Principal Editor, and other contributions preferably to a Specialist Editor in the appropriate field or to one who is geographically convenient. All manuscripts must be in English and should be typewritten double-spaced with wide margins on good quality A4 or $8.5 \times 11$ in.$^2$ ($21.6 \times 28$ cm$^2$) paper. Figures must be suitable for direct photographic reproduction. Sections should be decimally numbered, and references indicated in the text consecutively by Arabic numerals in square brackets.

### Programs

The manuscript for a program consists of the following (in duplicate):

(i) Program Summary *.

(ii) Long Write-up – a detailed description of the program: problem, method of solution, program design (with a flow diagram), operating instructions, input data, output (including error diagnostics), and the input data and selected output of up to three test runs. References should include a definition of the programming language if other than FORTRAN IV, FORTRAN 77 or ALGOL 60,

together with one copy each of:

(iii) Program Listings – the complete output from a compile–load–go job which adequately tests the program by means of up to three test runs. Not more than three pages of selected test results should be indicated for photographic reproduction in the journal to provide a check for the user and the printing should be clear enough to allow good reproduction. The complete input deck including all job control and input data cards should be numbered consecutively in columns 77–80 starting with 0001. Columns 73–76 should be left blank. After acceptance for publication the Author will be asked to send this deck to the Program Library preferably on magnetic tape.

(iv) Test Run Output – separate copies of the test results in a form suitable for direct reproduction in the journal. Photographs of output from a high-quality printer or terminal are preferred.

### Program adaptations

The manuscript to describe briefly an adaptation of a published program consists (in duplicate) of:

(i) Adaptation Summary *.

(ii) Long Write-up,

together with one copy each of:

(iii) Listing of the adaptation deck – this consecutively numbered deck will later be required by the Program Library and consists of "new" statements plus comments to explain by reference to card numbers, how to modify the program deck.

(iv) Complete listing from a compile–load–go job with the modified program including test input data and selected results.

(v) Test Run Output.

### Erratum notices

The manuscript to describe corrections to a published write-up and/or program consists (in duplicate) of:

(i) Erratum Summary *.

(ii) Explanation of corrections and if the program itself has been modified: one copy each of:

(iii) Listing of the deck – this consecutively numbered deck will later be required by the Program Library and consists of "new" statements plus comments to explain, by reference to card numbers, how to modify the program deck.

(iv) Complete listing from a compile–load–go job with the modified program including test input data and selected results.

### Proof correction

Corrections other than the printers' errors may be charged for.

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* A more detailed version of the Instructions of Authors and summary forms are available from the Principal Editor and are printed in Comput. Phys. Commun. 27 (1982) 1–9.

† A description of the Library is given in Comput. Phys. Commun. 19 (1980) 11–15. A complete index of programs is available from the Program Library.

## COMPUTER PHYSICS COMMUNICATIONS

Volume 35 (MASTER INDEX) December 1984

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